



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 01:18 PM EST

PDB ID : 6CFK  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with D-histidyl-CAM and bound to protein Y (YfiA) at 2.7Å resolution  
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.  
Deposited on : 2018-02-15  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)

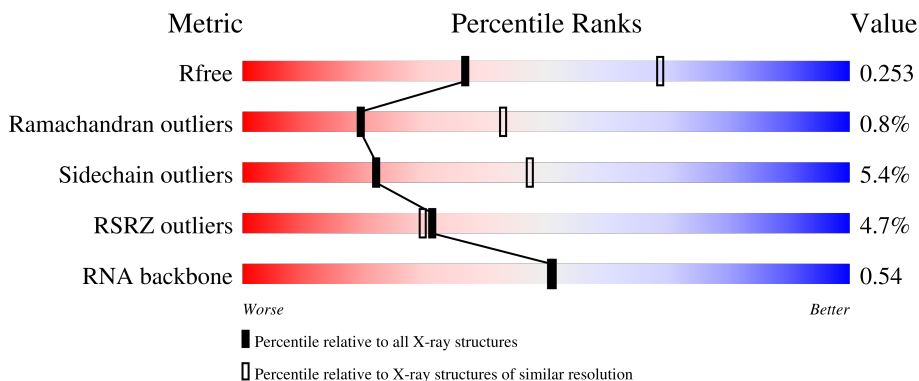
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


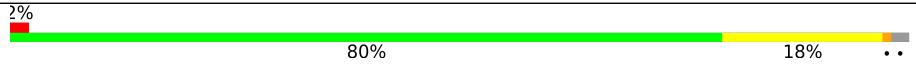

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2808 (2.70-2.70)                                      |
| Ramachandran outliers | 138981                      | 3069 (2.70-2.70)                                      |
| Sidechain outliers    | 138945                      | 3069 (2.70-2.70)                                      |
| RSRZ outliers         | 127900                      | 2737 (2.70-2.70)                                      |
| RNA backbone          | 3102                        | 1159 (3.00-2.40)                                      |


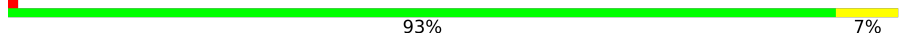




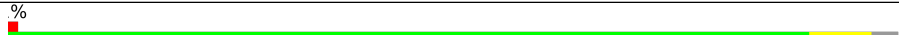
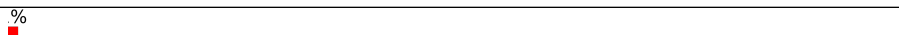
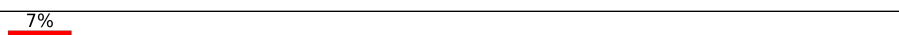
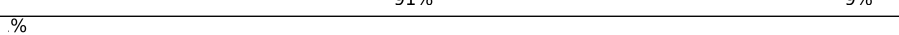
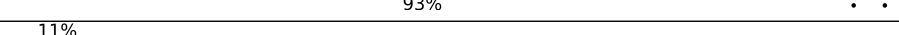
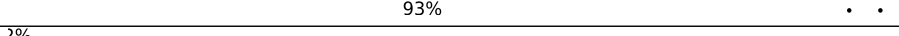
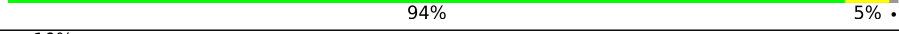
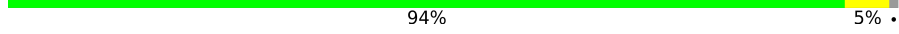
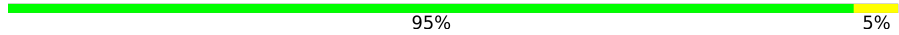
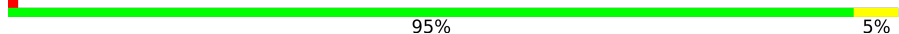
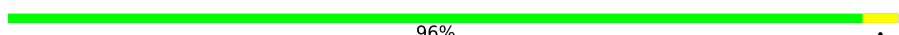
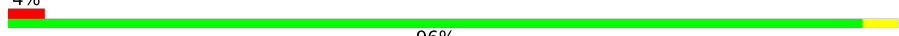





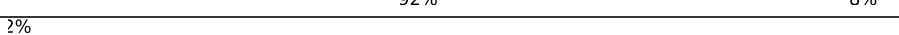

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 1A    | 2915   | <br>2% 82% 15% .. |
| 1   | 2A    | 2915   | <br>2% 80% 18% .. |
| 2   | 1B    | 121    | <br>89% 10% .     |

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.36

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | 2B    | 121    |  84% 15%   |
| 3   | 1D    | 276    |  93% 7%    |
| 3   | 2D    | 276    |  93% 7%    |
| 4   | 1E    | 206    |  92% 7%    |
| 4   | 2E    | 206    |  94% 5%    |
| 5   | 1F    | 210    |  89% 8%    |
| 5   | 2F    | 210    |  90% 7%    |
| 6   | 1G    | 182    |  93% 6%    |
| 6   | 2G    | 182    |  91% 9%    |
| 7   | 1H    | 180    |  93%       |
| 7   | 2H    | 180    |  93%       |
| 8   | 1I    | 148    |  94% 5%    |
| 8   | 2I    | 148    |  94% 5%   |
| 9   | 1N    | 140    |  95% 5%  |
| 9   | 2N    | 140    |  95% 5%  |
| 10  | 1O    | 122    |  96%     |
| 10  | 2O    | 122    |  96%     |
| 11  | 1P    | 150    |  97%     |
| 11  | 2P    | 150    |  95%     |
| 12  | 1Q    | 141    |  94% 6%  |
| 12  | 2Q    | 141    |  96%     |
| 13  | 1R    | 118    |  92% 8%  |
| 13  | 2R    | 118    |  89% 11% |
| 14  | 1S    | 112    |  92% 5%  |
| 14  | 2S    | 112    |  93% 5%  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | 1T    | 146    | 86% 10%          |
| 15  | 2T    | 146    | 86% 10%          |
| 16  | 1U    | 118    | 94%              |
| 16  | 2U    | 118    | 96% 8%           |
| 17  | 1V    | 101    | 92% 7%           |
| 17  | 2V    | 101    | 96% 3%           |
| 18  | 1W    | 113    | 91% 8%           |
| 18  | 2W    | 113    | 92% 7%           |
| 19  | 1X    | 96     | 93% 6%           |
| 19  | 2X    | 96     | 94% 5%           |
| 20  | 1Y    | 110    | 92% 5%           |
| 20  | 2Y    | 110    | 95% 14%          |
| 21  | 1Z    | 206    | 91% 7%           |
| 21  | 2Z    | 206    | 94%              |
| 22  | 10    | 85     | 86% 5% 9%        |
| 22  | 20    | 85     | 88% 9%           |
| 23  | 11    | 98     | 95%              |
| 23  | 21    | 98     | 95%              |
| 24  | 12    | 72     | 96%              |
| 24  | 22    | 72     | 96%              |
| 25  | 13    | 60     | 90% 8%           |
| 25  | 23    | 60     | 93% 5%           |
| 26  | 14    | 71     | 89% 8%           |
| 26  | 24    | 71     | 89% 8%           |
| 27  | 15    | 60     | 85% 13%          |

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| Mol | Chain | Length | Quality of chain        |
|-----|-------|--------|-------------------------|
| 27  | 25    | 60     | 3%<br>92%<br>7%         |
| 28  | 16    | 54     | 89%<br>9%               |
| 28  | 26    | 54     | 91%<br>7%               |
| 29  | 17    | 49     | 4%<br>88%<br>10%        |
| 29  | 27    | 49     | 8%<br>98%               |
| 30  | 18    | 65     | 2%<br>92%<br>6%         |
| 30  | 28    | 65     | 6%<br>91%<br>8%         |
| 31  | 19    | 37     | 3%<br>95%<br>5%         |
| 31  | 29    | 37     | 22%<br>97%              |
| 32  | 1a    | 1521   | %<br>82%<br>16%         |
| 32  | 2a    | 1521   | 2%<br>80%<br>18%        |
| 33  | 1b    | 256    | 4%<br>83%<br>7%<br>10%  |
| 33  | 2b    | 256    | 13%<br>84%<br>6%<br>10% |
| 34  | 1c    | 239    | 5%<br>84%<br>14%        |
| 34  | 2c    | 239    | 13%<br>82%<br>14%       |
| 35  | 1d    | 209    | 10%<br>95%<br>5%        |
| 35  | 2d    | 209    | 19%<br>96%              |
| 36  | 1e    | 162    | 2%<br>88%<br>9%         |
| 36  | 2e    | 162    | 12%<br>88%<br>9%        |
| 37  | 1f    | 101    | %<br>96%                |
| 37  | 2f    | 101    | 96%                     |
| 38  | 1g    | 156    | 4%<br>97%               |
| 38  | 2g    | 156    | 6%<br>94%<br>5%         |
| 39  | 1h    | 138    | 6%<br>98%               |
| 39  | 2h    | 138    | 5%<br>95%               |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 40  | 1i    | 128    | 13%<br>98% ..     |
| 40  | 2i    | 128    | 38%<br>94% 5% .   |
| 41  | 1j    | 105    | 12%<br>88% 5% 8%  |
| 41  | 2j    | 105    | 45%<br>89% . 9%   |
| 42  | 1k    | 129    | 85% . 12%         |
| 42  | 2k    | 129    | 5%<br>84% . 12%   |
| 43  | 1l    | 132    | 3%<br>89% . 8%    |
| 43  | 2l    | 132    | 12%<br>90% . 8%   |
| 44  | 1m    | 126    | 3%<br>87% 5% 8%   |
| 44  | 2m    | 126    | 10%<br>87% . 10%  |
| 45  | 1n    | 61     | 16%<br>97% ..     |
| 45  | 2n    | 61     | 59%<br>98% .      |
| 46  | 1o    | 89     | 91% 8% .          |
| 46  | 2o    | 89     | 2%<br>97% ..      |
| 47  | 1p    | 88     | 14%<br>88% 6% 7%  |
| 47  | 2p    | 88     | 9%<br>85% 8% 7%   |
| 48  | 1q    | 105    | 6%<br>90% 5% 6%   |
| 48  | 2q    | 105    | 7%<br>90% 5% 6%   |
| 49  | 1r    | 88     | %<br>76% . 23%    |
| 49  | 2r    | 88     | 2%<br>70% 7% 23%  |
| 50  | 1s    | 93     | %<br>86% . 11%    |
| 50  | 2s    | 93     | 16%<br>87% . 11%  |
| 51  | 1t    | 106    | 14%<br>85% 6% 9%  |
| 51  | 2t    | 106    | 7%<br>85% 7% . 8% |
| 52  | 1u    | 27     | 33%<br>81% . 15%  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | 2u    | 27     |                  |
| 53  | 1y    | 113    |                  |
| 53  | 2y    | 113    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | MG   | 1A    | 3189 | -         | -        | -       | X                |
| 54  | MG   | 1A    | 3921 | -         | -        | -       | X                |
| 54  | MG   | 1F    | 311  | -         | -        | -       | X                |
| 54  | MG   | 1a    | 1767 | -         | -        | -       | X                |
| 54  | MG   | 1a    | 1851 | -         | -        | -       | X                |
| 54  | MG   | 2A    | 3146 | -         | -        | -       | X                |
| 54  | MG   | 2A    | 3206 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 295438 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
|     |       |          | Total | C     | N     | O     | P    |         |         |       |
| 1   | 1A    | 2872     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61869 | 27540 | 11574 | 19884 | 2871 |         |         |       |
| 1   | 2A    | 2867     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61758 | 27491 | 11552 | 19850 | 2865 |         |         |       |

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | P   |         |         |       |
| 2   | 1B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2572  | 1145 | 476 | 832 | 119 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |         |       |
| 3   | 1D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2131  | 1346 | 422 | 360 | 3 |         |         |       |
| 3   | 2D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 4   | 1E    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |
| 4   | 2E    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L4.



| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | 1F    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1584  | 1009 | 298 | 275 | 2 |         |         |       |
| 5   | 2F    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1580  | 1007 | 297 | 274 | 2 |         |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | 1G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 916 | 253 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 912 | 259 | 249 | 4 |         |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | 1H    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |
| 7   | 2H    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1324  | 842 | 247 | 234 | 1 |         |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 1I    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1094  | 699 | 191 | 203 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 687 | 186 | 202 | 1 |         |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | 1N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 722 | 208 | 187 | 4 |         |         |       |
| 9   | 2N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | 1O    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 10  | 2O    | 122      | 933   | 588 | 171 | 170 | 4 | 0       | 0       | 0     |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 11  | 1P    | 149      | 1135  | 706 | 230 | 196 | 3 | 0       | 0       | 0     |
| 11  | 2P    | 149      | 1135  | 706 | 230 | 196 | 3 | 0       | 0       | 0     |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 12  | 1Q    | 141      | 1122  | 715 | 212 | 188 | 7 | 0       | 0       | 0     |
| 12  | 2Q    | 141      | 1122  | 715 | 212 | 188 | 7 | 0       | 0       | 0     |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 13  | 1R    | 118      | 968   | 604 | 203 | 160 | 1 | 0       | 0       | 0     |
| 13  | 2R    | 118      | 968   | 604 | 203 | 160 | 1 | 0       | 0       | 0     |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   |         |         |       |
| 14  | 1S    | 110      | 877   | 553 | 175 | 149 | 0       | 0       | 0     |
| 14  | 2S    | 110      | 870   | 549 | 173 | 148 | 0       | 0       | 0     |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 15  | 1T    | 131      | 1091  | 680 | 225 | 185 | 1 | 0       | 0       | 0     |
| 15  | 2T    | 131      | 1083  | 675 | 224 | 183 | 1 | 0       | 0       | 0     |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | 1U    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |
| 16  | 2U    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | 1V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 498 | 141 | 135 | 1 |         |         |       |
| 17  | 2V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | 1W    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |
| 18  | 2W    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | 1X    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |
| 19  | 2X    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | 1Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 520 | 153 | 131 | 6 |         |         |       |
| 20  | 2Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 519 | 153 | 132 | 6 |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 21  | 1Z    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1587  | 1011 | 282 | 292 | 2 |         |         |       |
| 21  | 2Z    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1557  | 995  | 274 | 286 | 2 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | 10    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |
| 22  | 20    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | 11    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 754   | 475 | 148 | 130 | 1 |         |         |       |
| 23  | 21    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 759   | 478 | 149 | 131 | 1 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | 12    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |
| 24  | 22    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 592   | 368 | 119 | 103 | 2 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 25  | 13    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 25  | 23    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 464   | 296 | 90 | 78 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 14    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 546   | 346 | 96 | 99 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 24    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 536   | 342 | 98 | 91 | 5 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | 15    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 27  | 25    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | 16    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |
| 28  | 26    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 279 | 91 | 75 | 4 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29  | 17    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 29  | 27    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30  | 18    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |
| 30  | 28    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | 19    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 31  | 29    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 32  | 1a    | 1500     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32246 | 14358 | 5975 | 10413 | 1500 |         |         |       |
| 32  | 2a    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32331 | 14396 | 5990 | 10441 | 1504 |         |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 33  | 1b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1842  | 1175 | 330 | 332 | 5 |         |         |       |
| 33  | 2b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1825  | 1167 | 326 | 327 | 5 |         |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | 1c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1558  | 979 | 305 | 273 | 1 |         |         |       |
| 34  | 2c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1542  | 968 | 300 | 273 | 1 |         |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35  | 1d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1665  | 1043 | 329 | 286 | 7 |         |         |       |
| 35  | 2d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1668  | 1047 | 330 | 284 | 7 |         |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | 1e    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |
| 36  | 2e    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | 1f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 814   | 516 | 144 | 151 | 3 |         |         |       |
| 37  | 2f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 146 | 151 | 3 |         |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | 1g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |
| 38  | 2g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1229  | 766 | 241 | 216 | 6 |         |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | 1h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1098  | 694 | 210 | 192 | 2 |         |         |       |
| 39  | 2h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40  | 1i    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 986   | 625 | 193 | 168 |         |         |       |
| 40  | 2i    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 966   | 613 | 186 | 167 |         |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41  | 1j    | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 719   | 446 | 142 | 131 |         |         |       |
| 41  | 2j    | 96       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 710   | 442 | 137 | 131 |         |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | 1k    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 520 | 156 | 155 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 42  | 2k    | 114      | 833   | 519 | 156 | 155 | 3 | 0       | 0       | 0     |

- Molecule 43 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 43  | 1l    | 122      | 932   | 586 | 185 | 159 | 2 | 0       | 0       | 0     |
| 43  | 2l    | 122      | 932   | 586 | 185 | 159 | 2 | 0       | 0       | 0     |

- Molecule 44 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 44  | 1m    | 116      | 914   | 564 | 189 | 159 | 2 | 0       | 0       | 0     |
| 44  | 2m    | 114      | 895   | 550 | 186 | 157 | 2 | 0       | 0       | 0     |

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |         |       |
| 45  | 1n    | 60       | 492   | 312 | 104 | 72 | 4 | 0       | 0       | 0     |
| 45  | 2n    | 60       | 492   | 312 | 104 | 72 | 4 | 0       | 0       | 0     |

- Molecule 46 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 46  | 1o    | 88       | 728   | 456 | 144 | 126 | 2 | 0       | 0       | 0     |
| 46  | 2o    | 88       | 728   | 456 | 144 | 126 | 2 | 0       | 0       | 0     |

- Molecule 47 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 47  | 1p    | 82       | 681   | 433 | 134 | 113 | 1 | 0       | 0       | 0     |
| 47  | 2p    | 82       | 677   | 430 | 133 | 113 | 1 | 0       | 0       | 0     |



- Molecule 48 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | 1q    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |
| 48  | 2q    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 49  | 1r    | 68       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |  |         |         |       |
| 49  | 2r    | 68       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |  |         |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | 1s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 415 | 120 | 111 | 2 |         |         |       |
| 50  | 2s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 410 | 118 | 115 | 2 |         |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | 1t    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 732   | 449 | 157 | 124 | 2 |         |         |       |
| 51  | 2t    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 451 | 154 | 126 | 2 |         |         |       |

- Molecule 52 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |   |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|---|
| 52  | 1u    | 23       | Total | C   | N  | O  |         | 0       | 0     | 0 |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |   |
| 52  | 2u    | 23       | Total | C   | N  | O  |         | 0       | 0     | 0 |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |   |

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | 1y    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 764   | 478 | 144 | 139 | 3 |         |         |       |
| 53  | 2y    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 749   | 468 | 141 | 137 | 3 |         |         |       |

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 54  | 1A    | 1024     | Total | Mg   | 0       | 0       |
|     |       |          | 1024  | 1024 |         |         |
| 54  | 1B    | 29       | Total | Mg   | 0       | 0       |
|     |       |          | 29    | 29   |         |         |
| 54  | 1D    | 13       | Total | Mg   | 0       | 0       |
|     |       |          | 13    | 13   |         |         |
| 54  | 1E    | 7        | Total | Mg   | 0       | 0       |
|     |       |          | 7     | 7    |         |         |
| 54  | 1F    | 13       | Total | Mg   | 0       | 0       |
|     |       |          | 13    | 13   |         |         |
| 54  | 1G    | 4        | Total | Mg   | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 54  | 1H    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 54  | 1N    | 3        | Total | Mg   | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 54  | 1O    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 54  | 1P    | 3        | Total | Mg   | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 54  | 1Q    | 4        | Total | Mg   | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 54  | 1R    | 3        | Total | Mg   | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 54  | 1S    | 1        | Total | Mg   | 0       | 0       |
|     |       |          | 1     | 1    |         |         |
| 54  | 1T    | 3        | Total | Mg   | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 54  | 1U    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 54  | 1V    | 3        | Total | Mg   | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 54  | 1W    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 54  | 1X    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |

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| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 54  | 1Z    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 10    | 6        | Total Mg<br>6 6     | 0       | 0       |
| 54  | 11    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 54  | 13    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 14    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 15    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 54  | 17    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 18    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 19    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 1a    | 255      | Total Mg<br>255 255 | 0       | 0       |
| 54  | 1b    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 1d    | 6        | Total Mg<br>6 6     | 0       | 0       |
| 54  | 1e    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 1f    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 1g    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 54  | 1h    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 1i    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 1l    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 1n    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 1o    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 1t    | 1        | Total Mg<br>1 1     | 0       | 0       |

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| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 54  | 1y    | 4        | Total Mg<br>4 4     | 0       | 0       |
| 54  | 2A    | 721      | Total Mg<br>721 721 | 0       | 0       |
| 54  | 2B    | 19       | Total Mg<br>19 19   | 0       | 0       |
| 54  | 2D    | 8        | Total Mg<br>8 8     | 0       | 0       |
| 54  | 2E    | 6        | Total Mg<br>6 6     | 0       | 0       |
| 54  | 2F    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 54  | 2G    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 54  | 2I    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2N    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2O    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2P    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 2Q    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 2R    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2T    | 4        | Total Mg<br>4 4     | 0       | 0       |
| 54  | 2V    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2W    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 2X    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 20    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 21    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 25    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 28    | 3        | Total Mg<br>3 3     | 0       | 0       |

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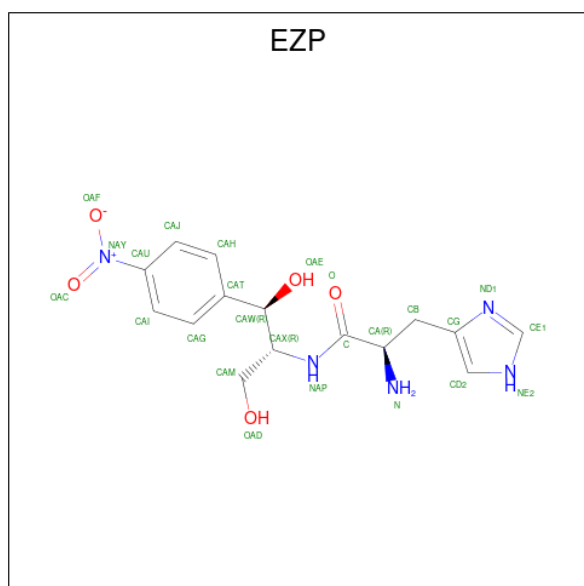
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| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 54  | 2a    | 151      | Total Mg<br>151 151 | 0       | 0       |
| 54  | 2e    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2f    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2j    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2p    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2q    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2r    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2t    | 1        | Total Mg<br>1 1     | 0       | 0       |

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

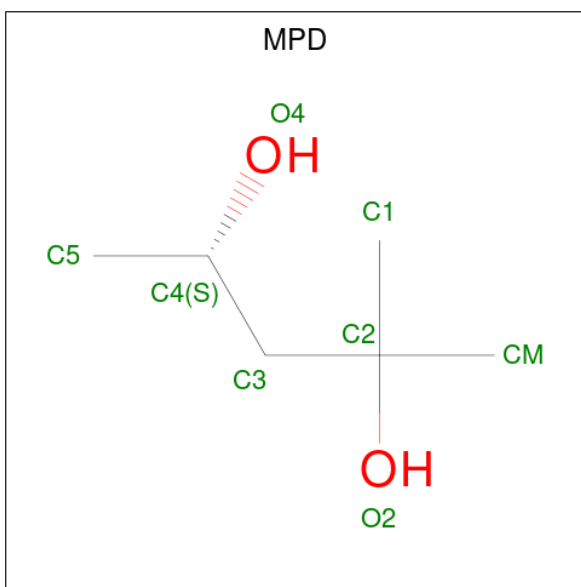
| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 55  | 1A    | 1        | Total K<br>1 1 | 0       | 0       |
| 55  | 2A    | 1        | Total K<br>1 1 | 0       | 0       |

- Molecule 56 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-D-histidinamide (three-letter code: EZP) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O<sub>5</sub>).



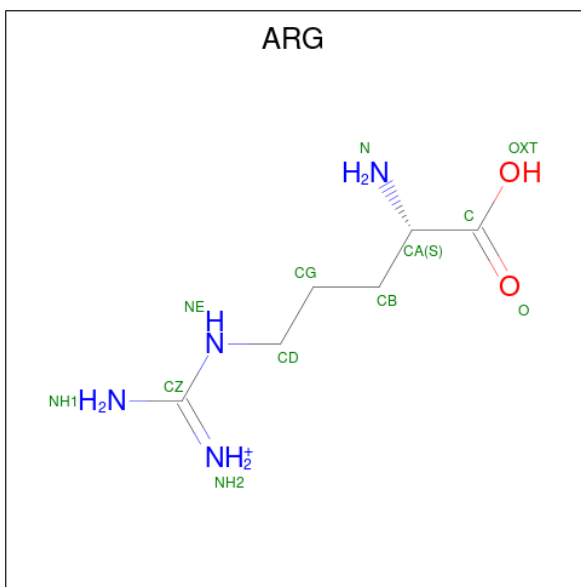
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 56  | 1A    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 25    | 15 | 5 | 5 |         |         |
| 56  | 2A    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 25    | 15 | 5 | 5 |         |         |

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 57  | 1A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 1T    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 18    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 1a    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 2A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 2A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 2B    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

- Molecule 58 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 58  | 1B    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 6 | 4 | 2 |         |         |
| 58  | 1F    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 6 | 4 | 2 |         |         |

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

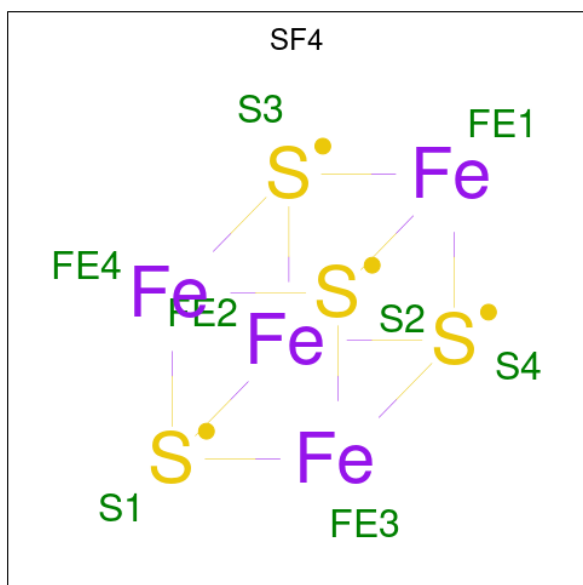
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | 1Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 2Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 24    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 25    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 26    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 59  | 29    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 59  | 2n    | 1        | Total Zn<br>1 1 | 0       | 0       |

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 60  | 1d    | 1        | Total Fe S<br>8 4 4 | 0       | 0       |
| 60  | 2d    | 1        | Total Fe S<br>8 4 4 | 0       | 0       |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 61  | 1A    | 2980     | Total O<br>2980 2980 | 0       | 0       |
| 61  | 1B    | 105      | Total O<br>105 105   | 0       | 0       |
| 61  | 1D    | 116      | Total O<br>116 116   | 0       | 0       |
| 61  | 1E    | 76       | Total O<br>76 76     | 0       | 0       |
| 61  | 1F    | 63       | Total O<br>63 63     | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 61  | 1G    | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 61  | 1H    | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 61  | 1I    | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 61  | 1N    | 50       | Total<br>50 | O<br>50 | 0       | 0       |
| 61  | 1O    | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 61  | 1P    | 58       | Total<br>58 | O<br>58 | 0       | 0       |
| 61  | 1Q    | 42       | Total<br>42 | O<br>42 | 0       | 0       |
| 61  | 1R    | 37       | Total<br>37 | O<br>37 | 0       | 0       |
| 61  | 1S    | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 61  | 1T    | 42       | Total<br>42 | O<br>42 | 0       | 0       |
| 61  | 1U    | 45       | Total<br>45 | O<br>45 | 0       | 0       |
| 61  | 1V    | 37       | Total<br>37 | O<br>37 | 0       | 0       |
| 61  | 1W    | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 61  | 1X    | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 61  | 1Y    | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 61  | 1Z    | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 61  | 10    | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 61  | 11    | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 61  | 12    | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 61  | 13    | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 61  | 14    | 2        | Total<br>2  | O<br>2  | 0       | 0       |

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| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 61  | 15    | 26       | Total O<br>26 26     | 0       | 0       |
| 61  | 16    | 17       | Total O<br>17 17     | 0       | 0       |
| 61  | 17    | 14       | Total O<br>14 14     | 0       | 0       |
| 61  | 18    | 30       | Total O<br>30 30     | 0       | 0       |
| 61  | 19    | 8        | Total O<br>8 8       | 0       | 0       |
| 61  | 1a    | 261      | Total O<br>261 261   | 0       | 0       |
| 61  | 1b    | 1        | Total O<br>1 1       | 0       | 0       |
| 61  | 1d    | 9        | Total O<br>9 9       | 0       | 0       |
| 61  | 1e    | 6        | Total O<br>6 6       | 0       | 0       |
| 61  | 1f    | 3        | Total O<br>3 3       | 0       | 0       |
| 61  | 1h    | 1        | Total O<br>1 1       | 0       | 0       |
| 61  | 1i    | 1        | Total O<br>1 1       | 0       | 0       |
| 61  | 1j    | 1        | Total O<br>1 1       | 0       | 0       |
| 61  | 1k    | 1        | Total O<br>1 1       | 0       | 0       |
| 61  | 1l    | 4        | Total O<br>4 4       | 0       | 0       |
| 61  | 1n    | 1        | Total O<br>1 1       | 0       | 0       |
| 61  | 1o    | 5        | Total O<br>5 5       | 0       | 0       |
| 61  | 1p    | 3        | Total O<br>3 3       | 0       | 0       |
| 61  | 1y    | 5        | Total O<br>5 5       | 0       | 0       |
| 61  | 2A    | 1686     | Total O<br>1686 1686 | 0       | 0       |
| 61  | 2B    | 65       | Total O<br>65 65     | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 61  | 2D    | 52       | Total<br>52 | O<br>52 | 0       | 0       |
| 61  | 2E    | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 61  | 2F    | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 61  | 2G    | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 61  | 2H    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 61  | 2I    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 61  | 2N    | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 61  | 2O    | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 61  | 2P    | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 61  | 2Q    | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 61  | 2R    | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 61  | 2S    | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 61  | 2T    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 61  | 2U    | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 61  | 2V    | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 61  | 2W    | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 61  | 2X    | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 61  | 2Y    | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 61  | 2Z    | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 61  | 20    | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 61  | 21    | 24       | Total<br>24 | O<br>24 | 0       | 0       |

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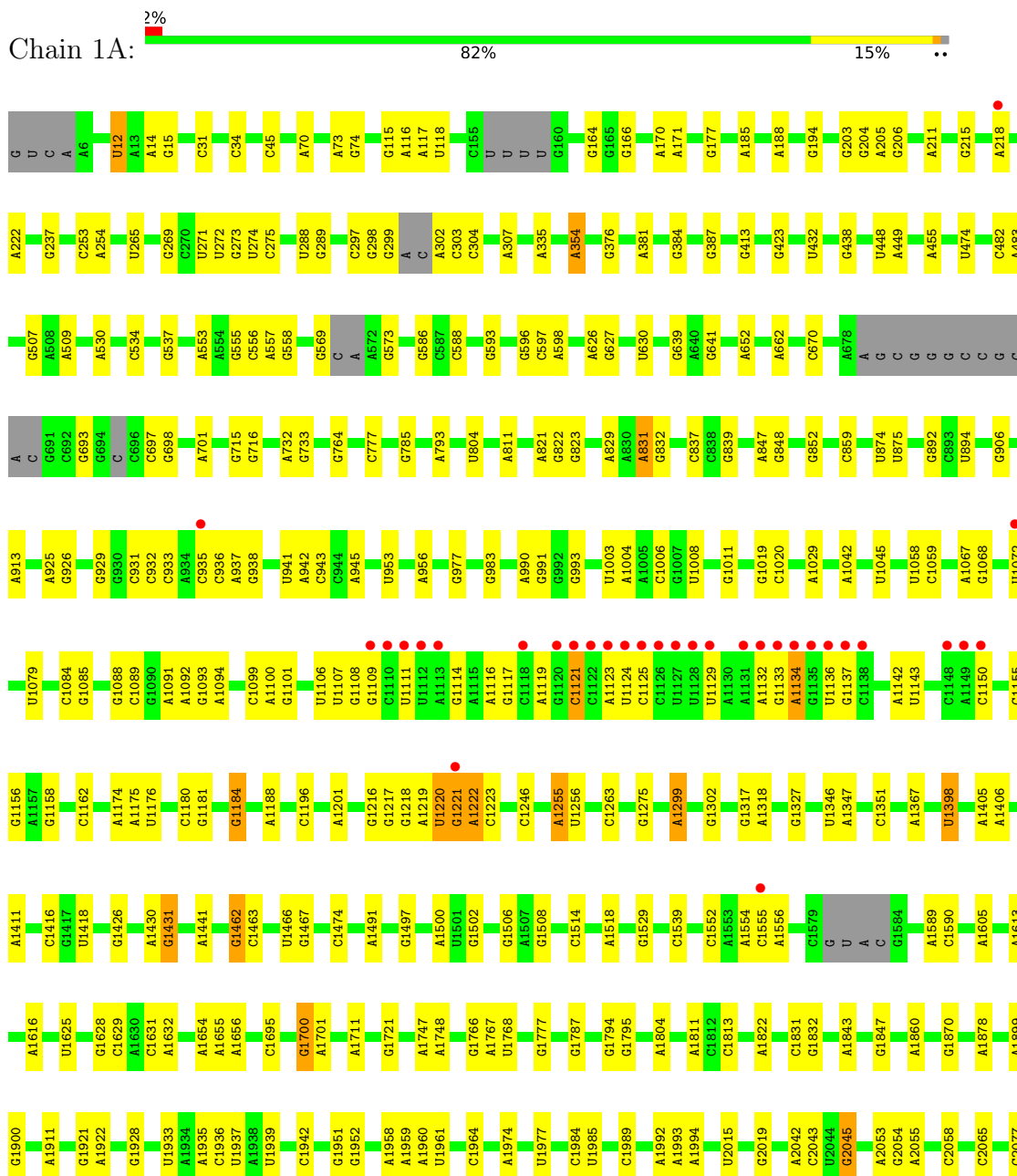
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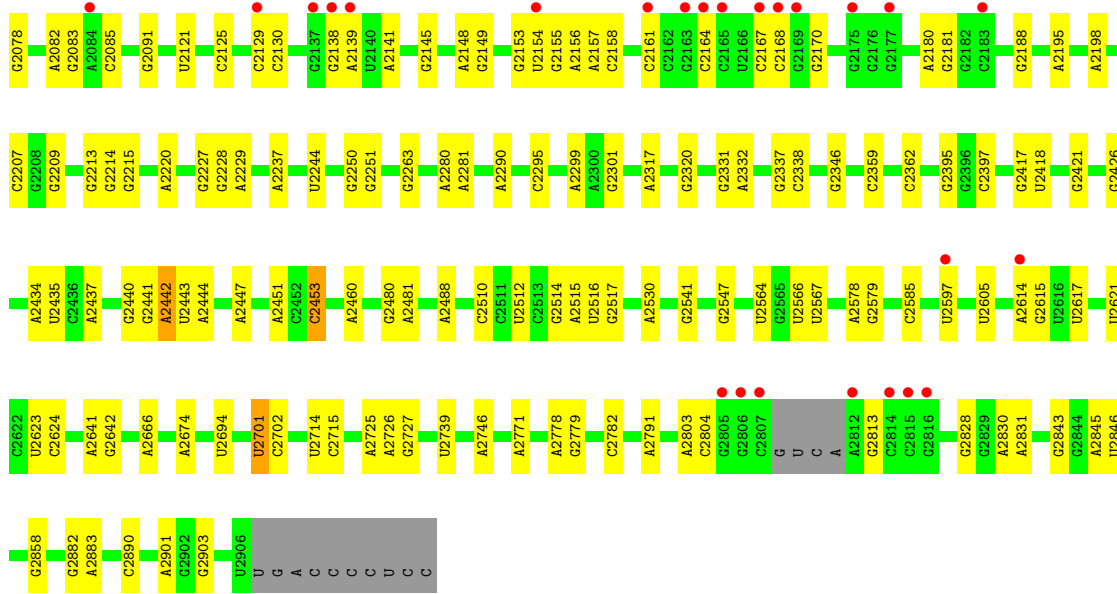
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 22    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | 23    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 24    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 25    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 61  | 26    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 61  | 27    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 61  | 28    | 15       | Total<br>15  | O<br>15  | 0       | 0       |
| 61  | 29    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2a    | 100      | Total<br>100 | O<br>100 | 0       | 0       |
| 61  | 2d    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 61  | 2e    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2f    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2j    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2l    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2m    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2o    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2p    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2q    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2r    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 2y    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

### 3 Residue-property plots [i](#)

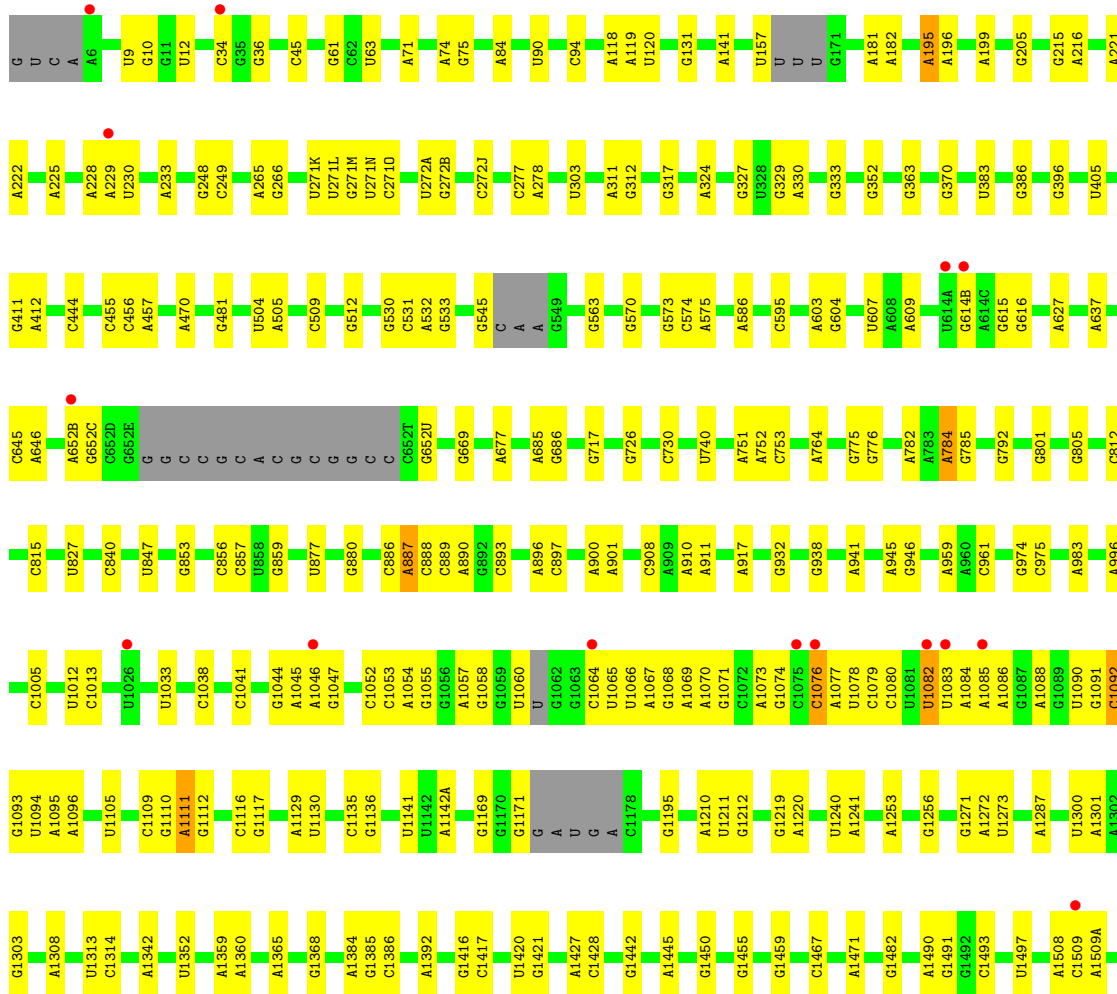
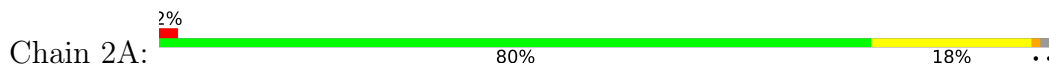
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

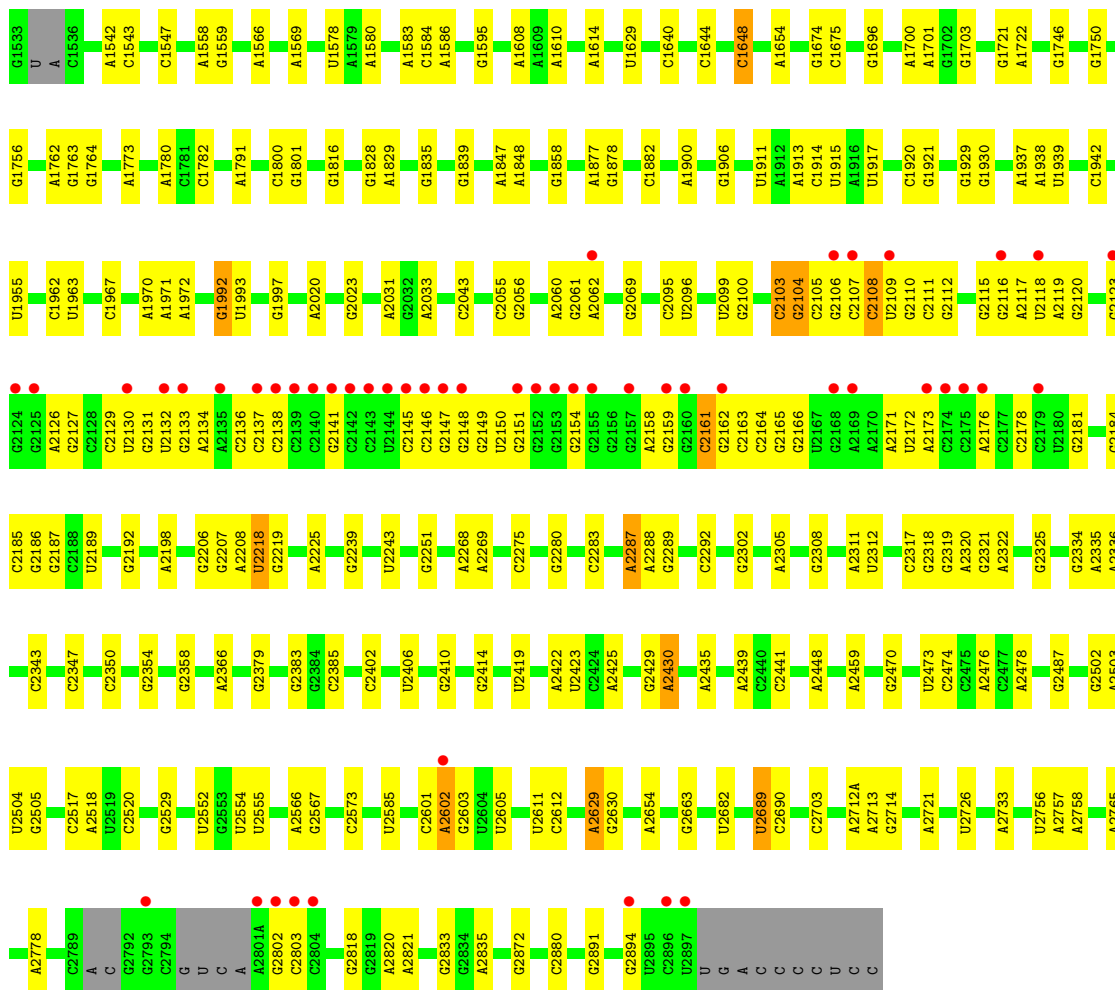
- Molecule 1: 23S Ribosomal RNA



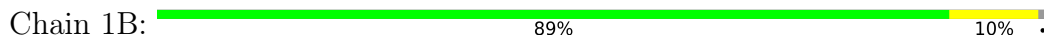


● Molecule 1: 23S Ribosomal RNA

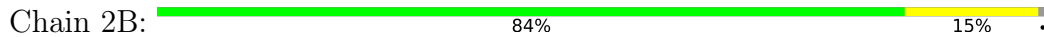




• Molecule 2: 5S Ribosomal RNA



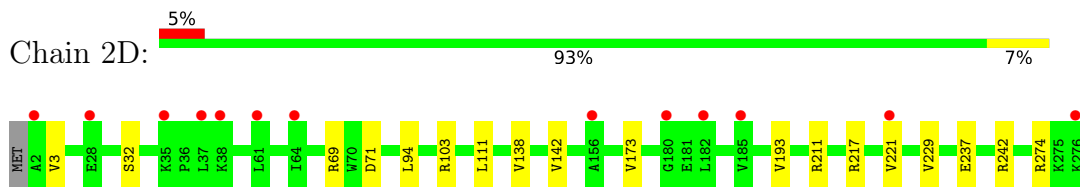
• Molecule 2: 5S Ribosomal RNA



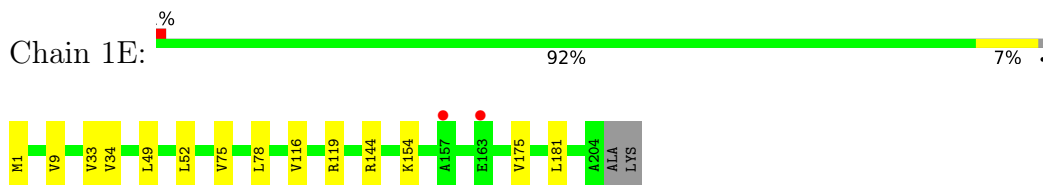
• Molecule 3: 50S ribosomal protein L2



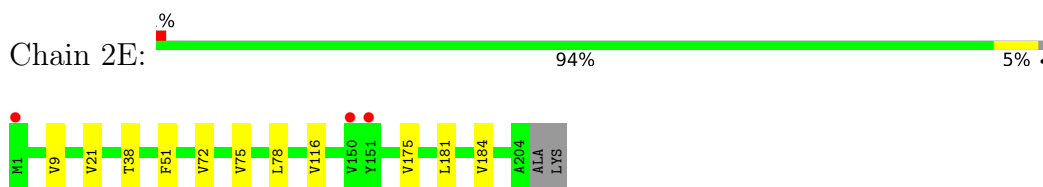
- Molecule 3: 50S ribosomal protein L2



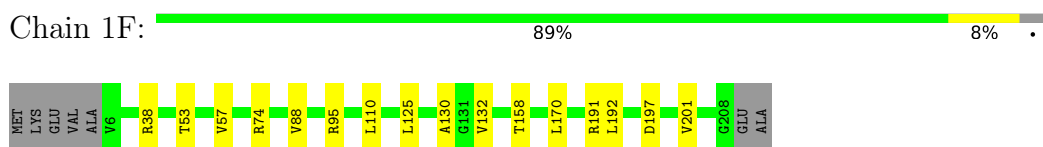
- Molecule 4: 50S ribosomal protein L3



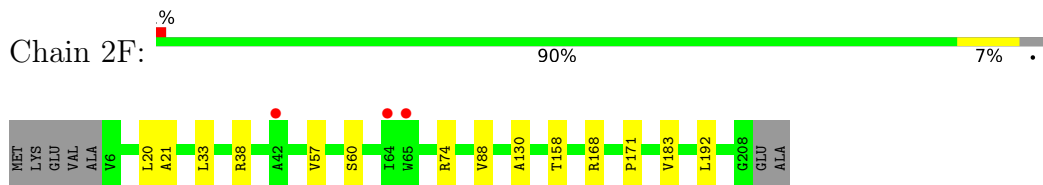
- Molecule 4: 50S ribosomal protein L3



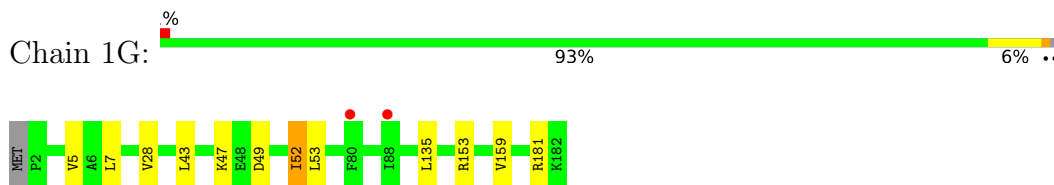
- Molecule 5: 50S ribosomal protein L4



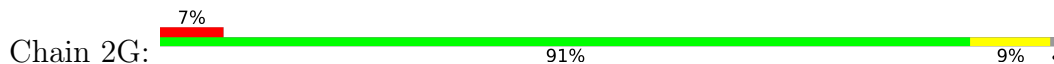
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5



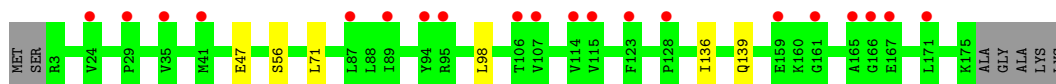




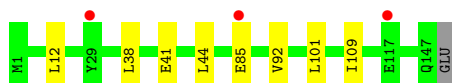
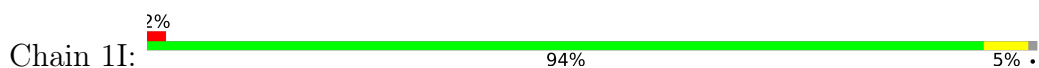
- Molecule 7: 50S ribosomal protein L6



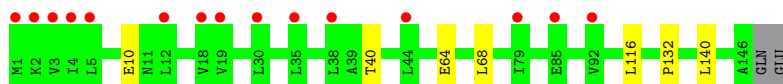
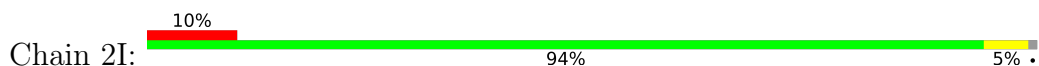
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



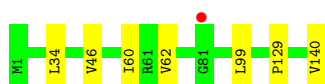
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

Chain 1O:  96%



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  96%



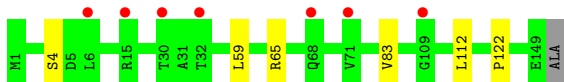
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  97%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  95%



- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  94%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  96%

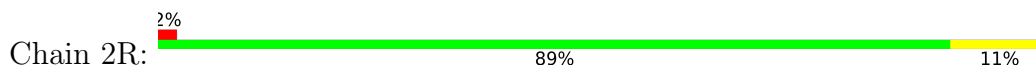


- Molecule 13: 50S ribosomal protein L17

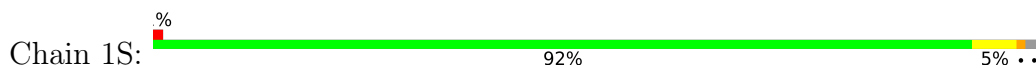
Chain 1R:  92%



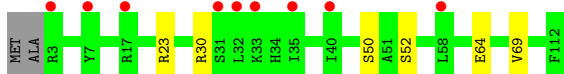
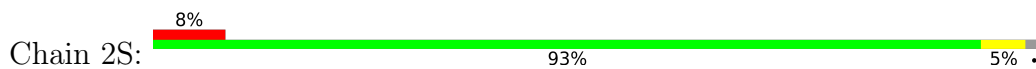
- Molecule 13: 50S ribosomal protein L17



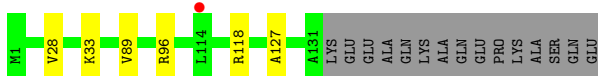
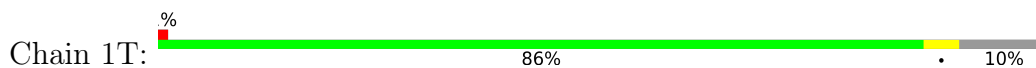
- Molecule 14: 50S ribosomal protein L18



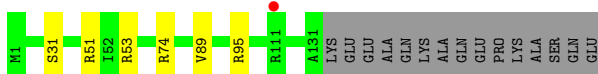
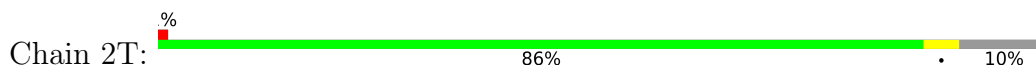
- Molecule 14: 50S ribosomal protein L18



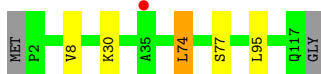
- Molecule 15: 50S ribosomal protein L19



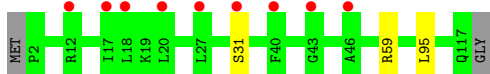
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

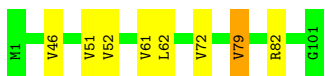


- Molecule 16: 50S ribosomal protein L20



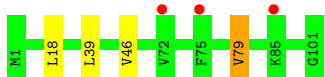
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  92% 7%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  96% 3%

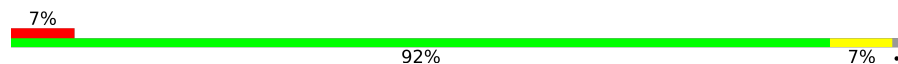


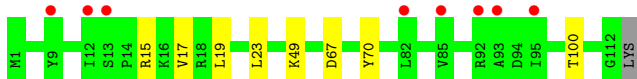
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  91% 8%



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  92% 7%



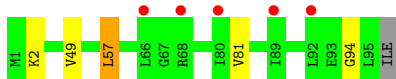
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  93% 6%



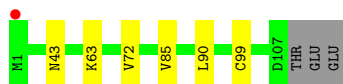
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  94% 5%

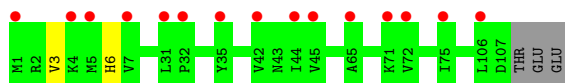


- Molecule 20: 50S ribosomal protein L24

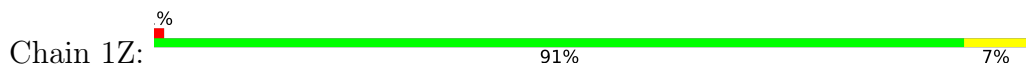
Chain 1Y:  92% 5%



- Molecule 20: 50S ribosomal protein L24



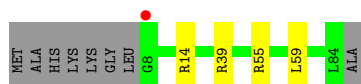
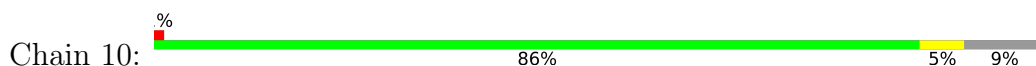
- Molecule 21: 50S ribosomal protein L25



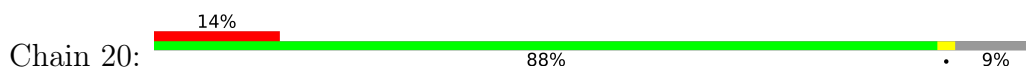
- Molecule 21: 50S ribosomal protein L25



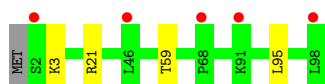
- Molecule 22: 50S ribosomal protein L27



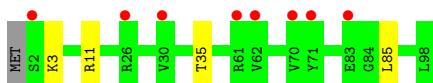
- Molecule 22: 50S ribosomal protein L27



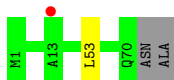
- Molecule 23: 50S ribosomal protein L28



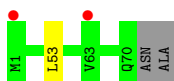
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



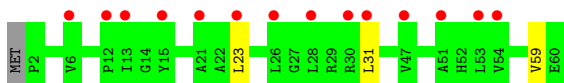
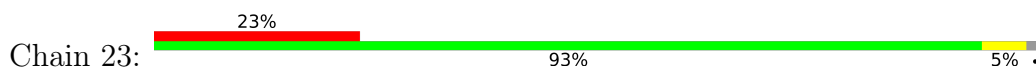
- Molecule 24: 50S ribosomal protein L29



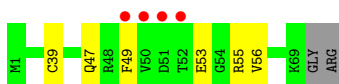
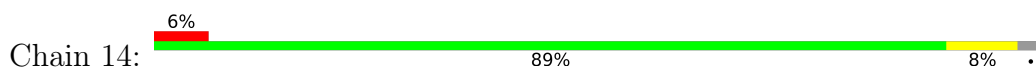
- Molecule 25: 50S ribosomal protein L30



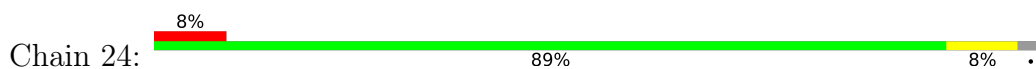
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31

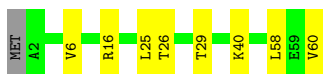


- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

Chain 15:  85% 13%




- Molecule 27: 50S ribosomal protein L32

Chain 25:  3% 92% 7%



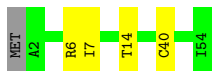
- Molecule 28: 50S ribosomal protein L33

Chain 16:  89% 9%




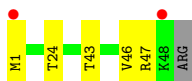
- Molecule 28: 50S ribosomal protein L33

Chain 26:  91% 7%



- Molecule 29: 50S ribosomal protein L34

Chain 17:  4% 88% 10%



- Molecule 29: 50S ribosomal protein L34

Chain 27:  8% 98%

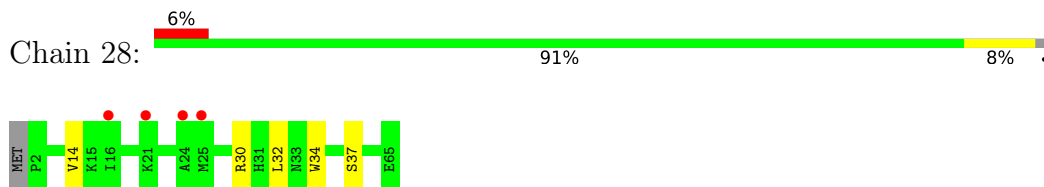


- Molecule 30: 50S ribosomal protein L35

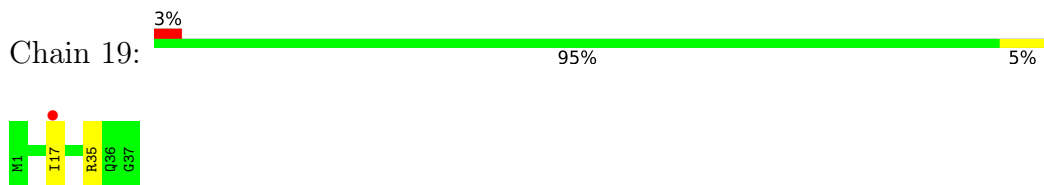
Chain 18:  2% 92% 6%



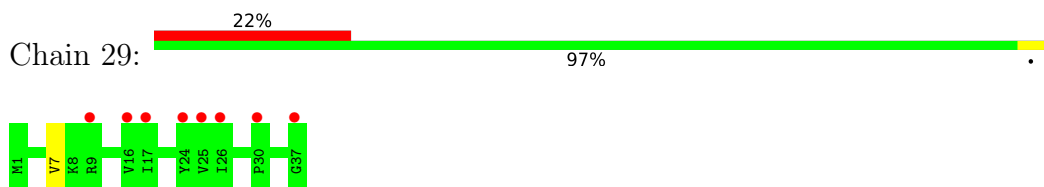
• Molecule 30: 50S ribosomal protein L35



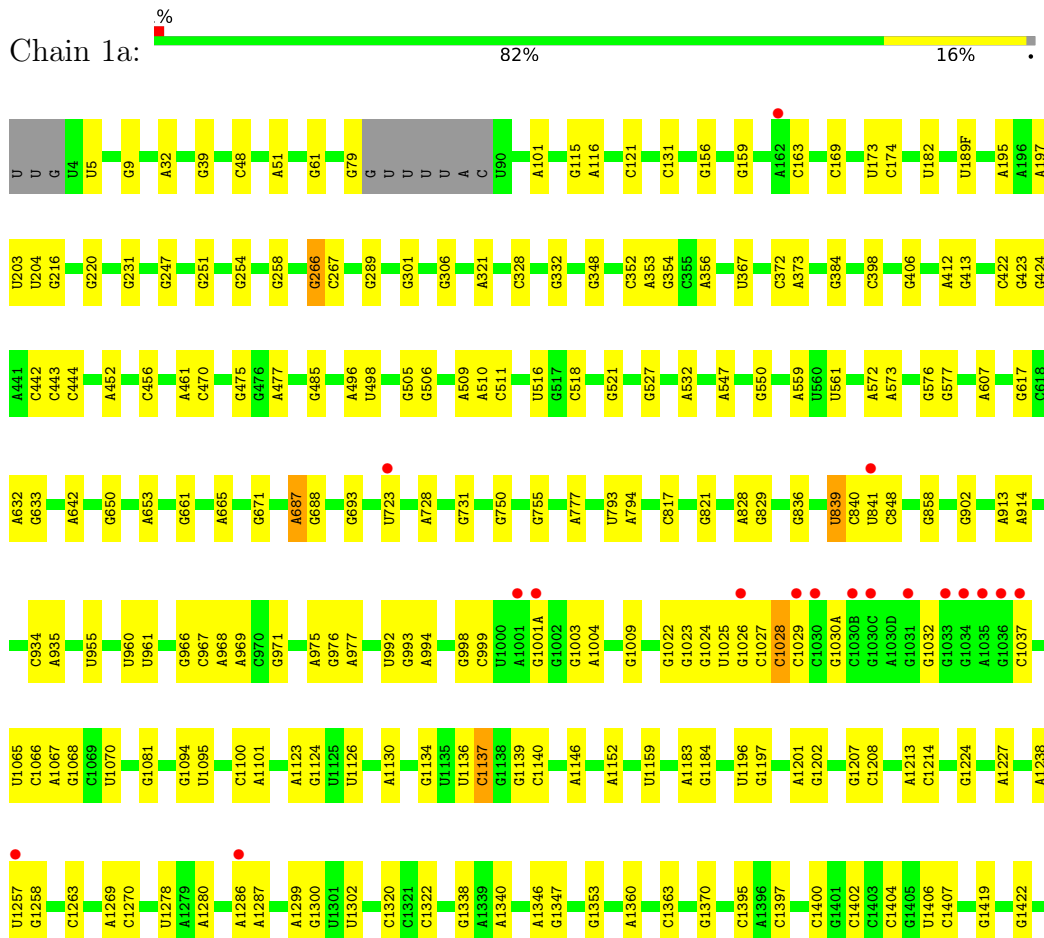
• Molecule 31: 50S ribosomal protein L36



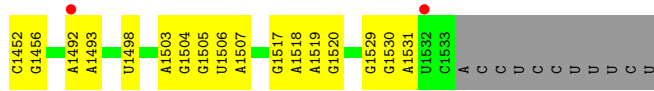
• Molecule 31: 50S ribosomal protein L36



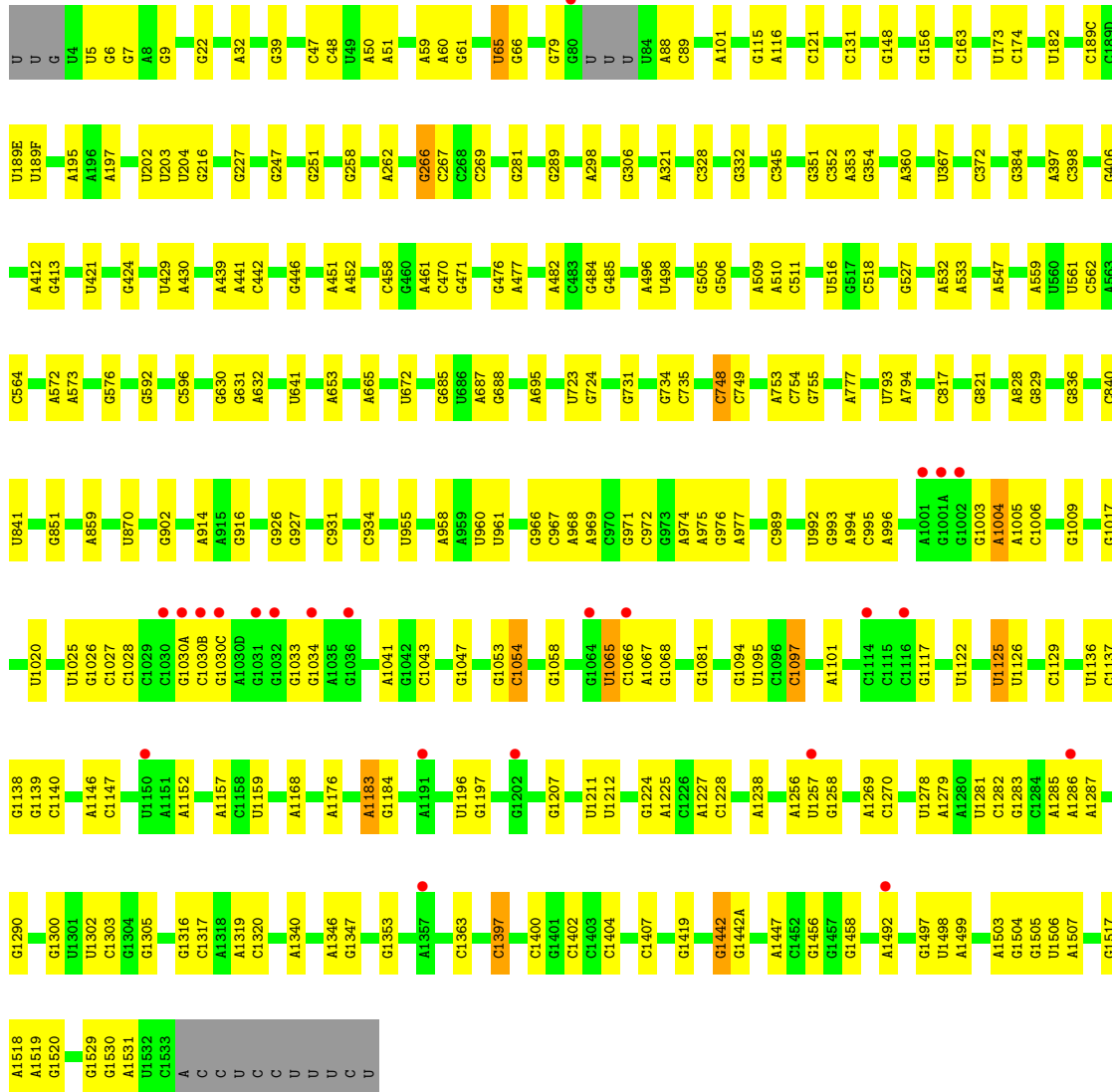
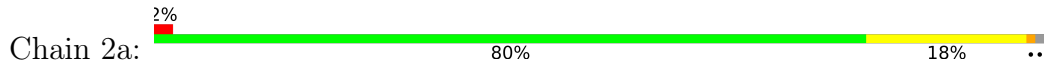
• Molecule 32: 16S Ribosomal RNA



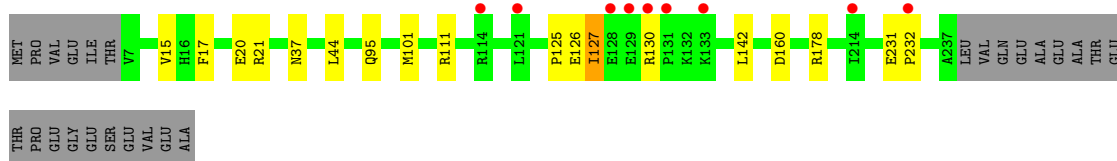
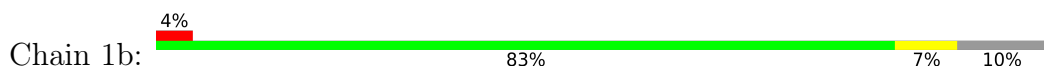




• Molecule 32: 16S Ribosomal RNA

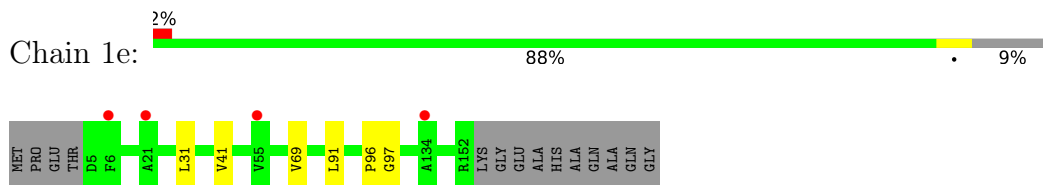


• Molecule 33: 30S ribosomal protein S2

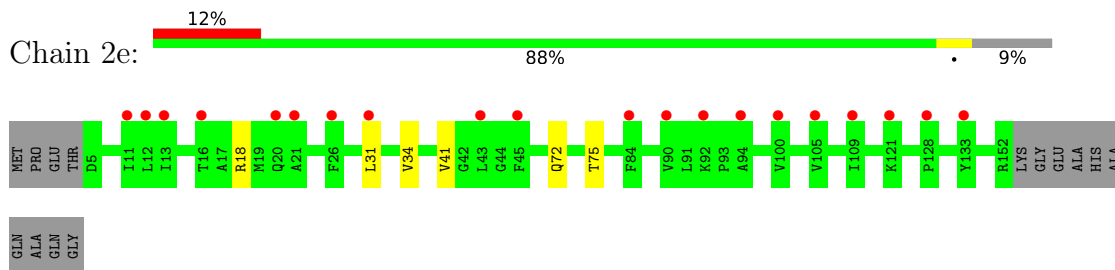




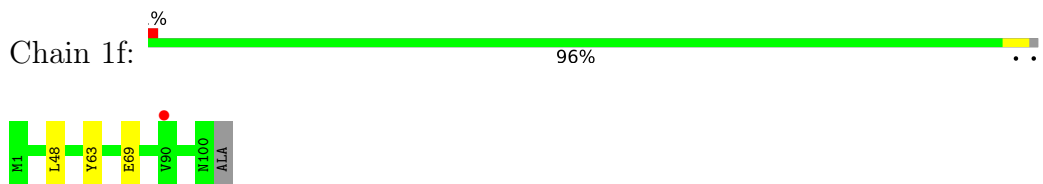
- Molecule 36: 30S ribosomal protein S5



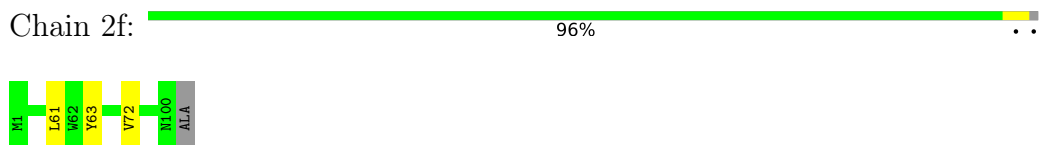
- Molecule 36: 30S ribosomal protein S5



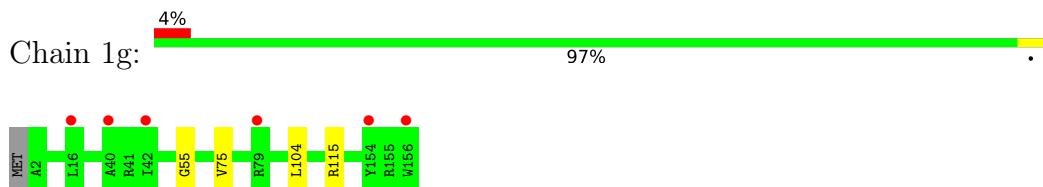
- Molecule 37: 30S ribosomal protein S6



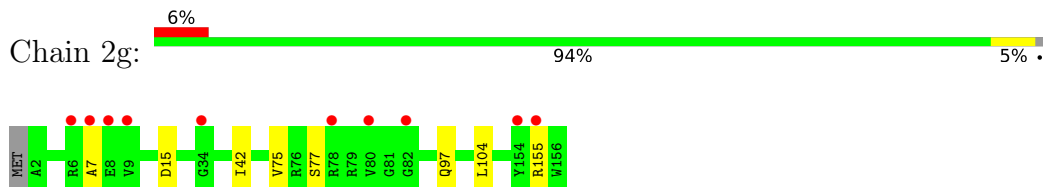
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

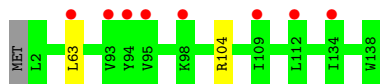


- Molecule 38: 30S ribosomal protein S7

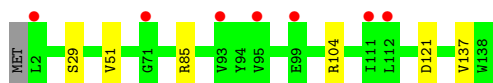


- Molecule 39: 30S ribosomal protein S8

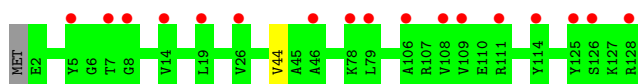




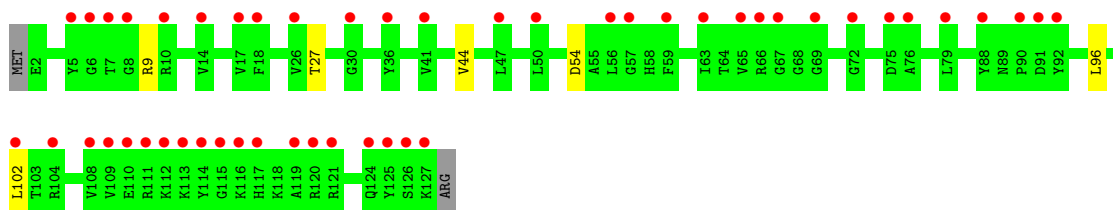
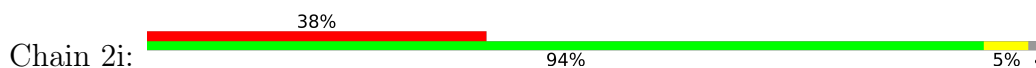
- Molecule 39: 30S ribosomal protein S8



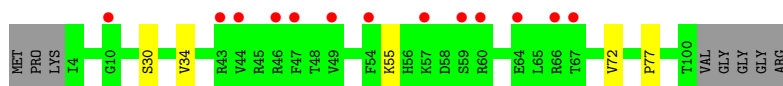
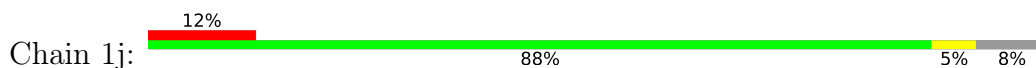
- Molecule 40: 30S ribosomal protein S9



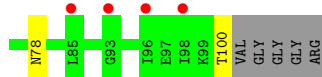
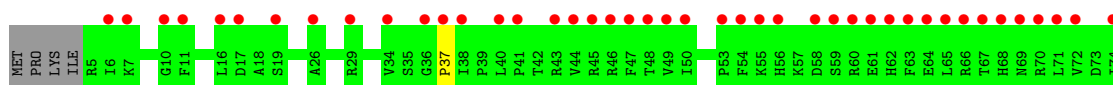
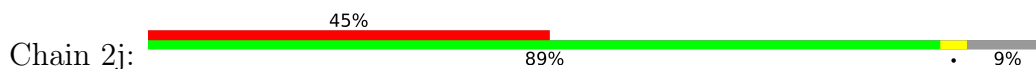
- Molecule 40: 30S ribosomal protein S9




- Molecule 41: 30S ribosomal protein S10

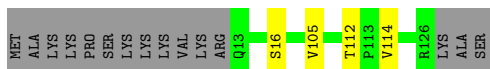


- Molecule 41: 30S ribosomal protein S10




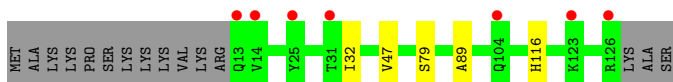
- Molecule 42: 30S ribosomal protein S11

Chain 1k:  85% 12%




• Molecule 42: 30S ribosomal protein S11

Chain 2k:  84% 12%




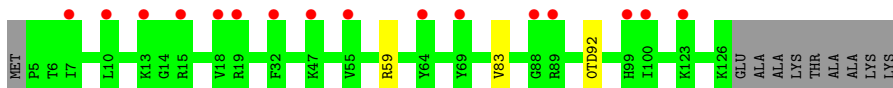
• Molecule 43: 30S ribosomal protein S12

Chain 1l:  89% 8%




• Molecule 43: 30S ribosomal protein S12

Chain 2l:  90% 8%

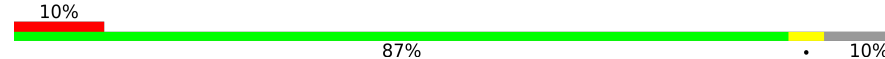


• Molecule 44: 30S ribosomal protein S13

Chain 1m:  87% 8%



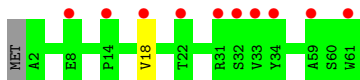
• Molecule 44: 30S ribosomal protein S13

Chain 2m:  87% 10%

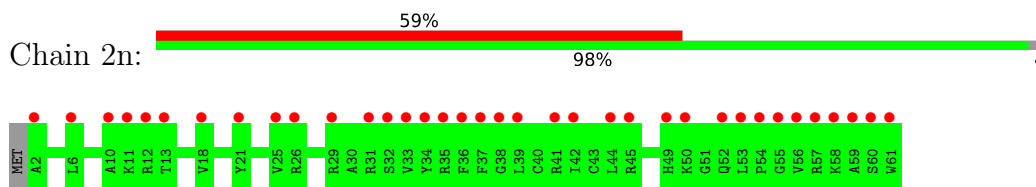


• Molecule 45: 30S ribosomal protein S14 type Z

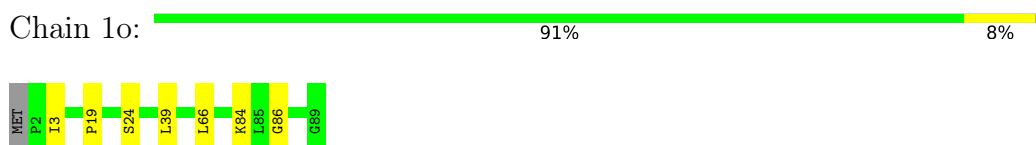
Chain 1n:  97%



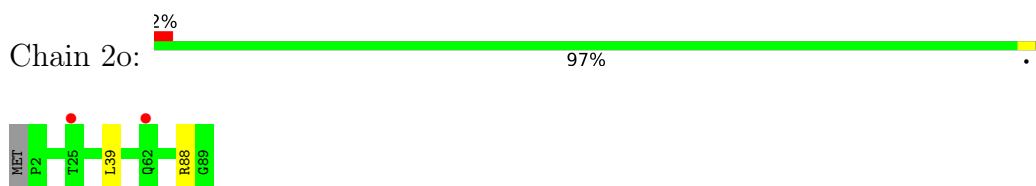
- Molecule 45: 30S ribosomal protein S14 type Z



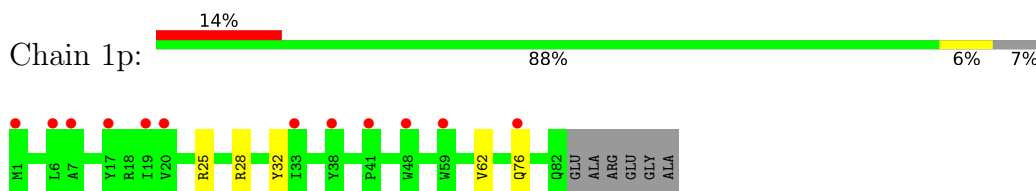
- Molecule 46: 30S ribosomal protein S15



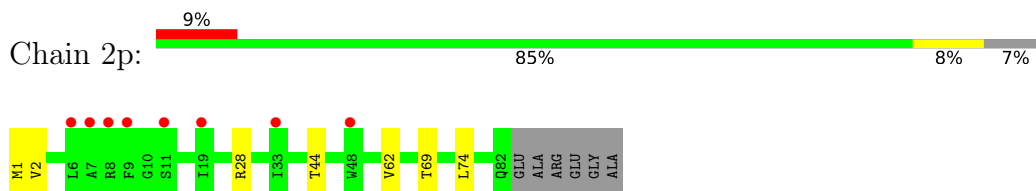
- Molecule 46: 30S ribosomal protein S15



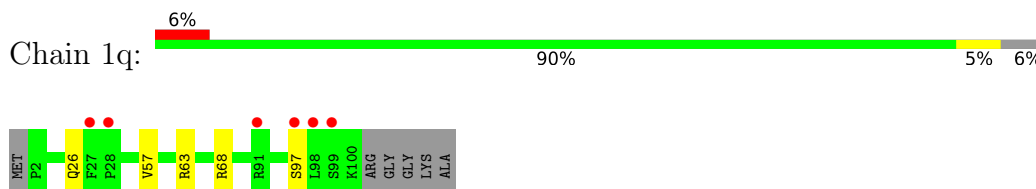
- Molecule 47: 30S ribosomal protein S16



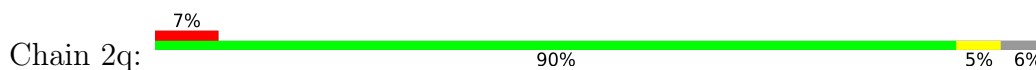
- Molecule 47: 30S ribosomal protein S16

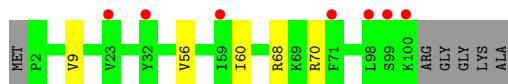


- Molecule 48: 30S ribosomal protein S17

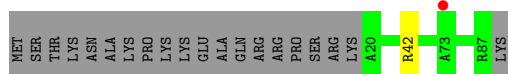
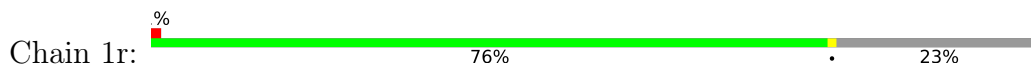


- Molecule 48: 30S ribosomal protein S17

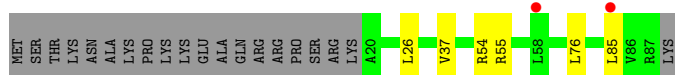




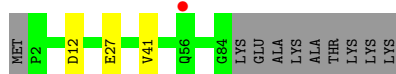
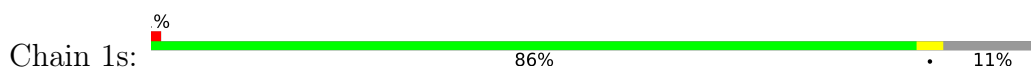
- Molecule 49: 30S ribosomal protein S18



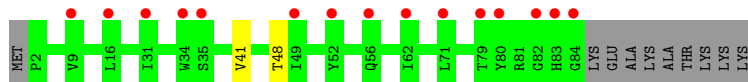
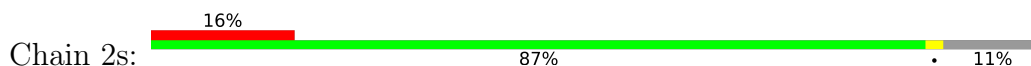
- Molecule 49: 30S ribosomal protein S18



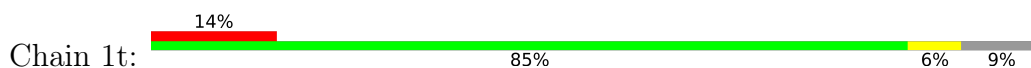
- Molecule 50: 30S ribosomal protein S19



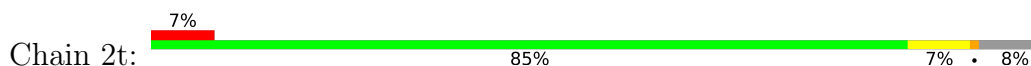
- Molecule 50: 30S ribosomal protein S19



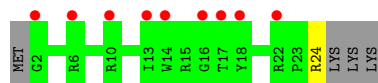
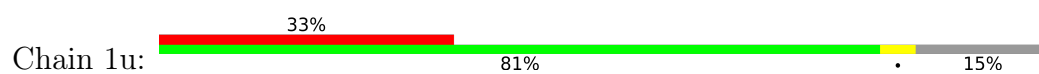
- Molecule 51: 30S ribosomal protein S20



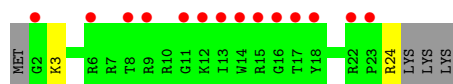
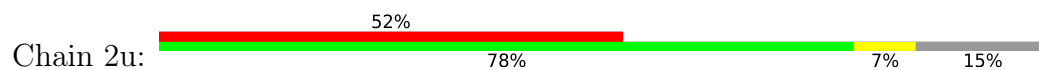
- Molecule 51: 30S ribosomal protein S20



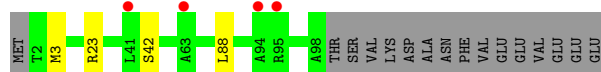
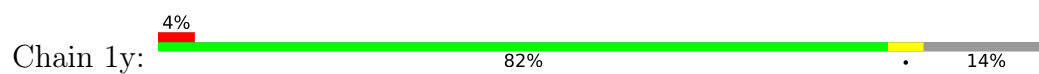
- Molecule 52: 30S ribosomal protein Thx



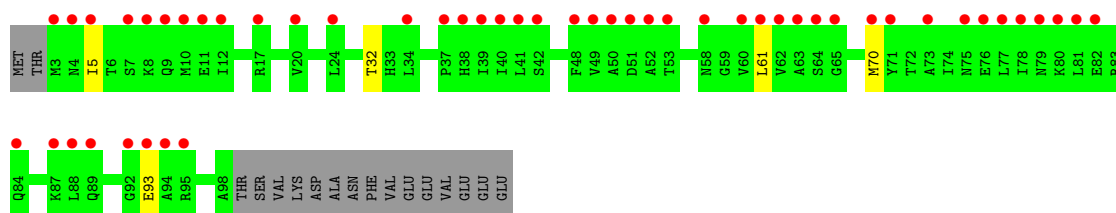
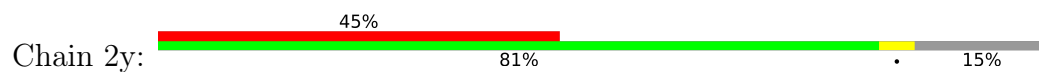
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.09Å 449.12Å 621.91Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 121.92 – 2.70<br>364.10 – 2.70                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (121.92-2.70)<br>99.2 (364.10-2.70)                    | Depositor<br>EDS |
| $R_{merge}$   | 0.15  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.24 (at 2.69Å)   | Xtrriage         |
| Refinement program  | PHENIX 1.8.2  | Depositor        |
| R, $R_{free}$   | 0.206 , 0.253<br>0.207 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set   | 79057 reflections (5.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 52.6  | Xtrriage         |
| Anisotropy  | 0.142   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 53.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 295438  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 54.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, MPD, K, 2MA, OMG, 2MU, EZP, M2G, 5MC, MG, 5MU, 7MG, SF4, PSU, 4OC, ZN, 2MG, 0TD, UR3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | 1A    | 0.51         | 0/69029 | 0.96        | 51/107746 (0.0%) |
| 1   | 2A    | 0.41         | 0/68901 | 0.90        | 41/107544 (0.0%) |
| 2   | 1B    | 0.43         | 0/2876  | 0.90        | 1/4486 (0.0%)    |
| 2   | 2B    | 0.37         | 0/2878  | 0.87        | 0/4490           |
| 3   | 1D    | 0.37         | 0/2181  | 0.59        | 0/2940           |
| 3   | 2D    | 0.33         | 0/2186  | 0.55        | 0/2944           |
| 4   | 1E    | 0.37         | 0/1592  | 0.55        | 0/2149           |
| 4   | 2E    | 0.31         | 0/1592  | 0.53        | 0/2149           |
| 5   | 1F    | 0.34         | 0/1619  | 0.53        | 0/2193           |
| 5   | 2F    | 0.31         | 0/1615  | 0.52        | 0/2188           |
| 6   | 1G    | 0.30         | 0/1451  | 0.50        | 0/1961           |
| 6   | 2G    | 0.30         | 0/1449  | 0.47        | 0/1957           |
| 7   | 1H    | 0.33         | 0/1356  | 0.51        | 0/1834           |
| 7   | 2H    | 0.29         | 0/1350  | 0.47        | 0/1826           |
| 8   | 1I    | 0.30         | 0/1109  | 0.52        | 0/1512           |
| 8   | 2I    | 0.28         | 0/1091  | 0.49        | 0/1490           |
| 9   | 1N    | 0.36         | 0/1148  | 0.55        | 0/1547           |
| 9   | 2N    | 0.29         | 0/1144  | 0.48        | 0/1543           |
| 10  | 1O    | 0.36         | 0/943   | 0.56        | 0/1269           |
| 10  | 2O    | 0.33         | 0/943   | 0.54        | 0/1269           |
| 11  | 1P    | 0.34         | 0/1152  | 0.57        | 0/1533           |
| 11  | 2P    | 0.32         | 0/1152  | 0.54        | 0/1533           |
| 12  | 1Q    | 0.35         | 0/1143  | 0.52        | 0/1527           |
| 12  | 2Q    | 0.30         | 0/1143  | 0.49        | 0/1527           |
| 13  | 1R    | 0.34         | 0/982   | 0.58        | 0/1312           |
| 13  | 2R    | 0.31         | 0/982   | 0.55        | 1/1312 (0.1%)    |
| 14  | 1S    | 0.31         | 0/887   | 0.52        | 0/1180           |
| 14  | 2S    | 0.30         | 0/880   | 0.50        | 0/1172           |
| 15  | 1T    | 0.33         | 0/1105  | 0.54        | 0/1477           |
| 15  | 2T    | 0.30         | 0/1097  | 0.51        | 0/1468           |
| 16  | 1U    | 0.36         | 0/977   | 0.53        | 1/1301 (0.1%)    |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 16  | 2U    | 0.30         | 0/977   | 0.45        | 0/1301          |
| 17  | 1V    | 0.34         | 0/786   | 0.54        | 0/1053          |
| 17  | 2V    | 0.32         | 0/782   | 0.52        | 0/1049          |
| 18  | 1W    | 0.33         | 0/897   | 0.51        | 0/1205          |
| 18  | 2W    | 0.32         | 0/897   | 0.50        | 0/1205          |
| 19  | 1X    | 0.38         | 0/764   | 0.56        | 0/1025          |
| 19  | 2X    | 0.31         | 0/764   | 0.55        | 1/1025 (0.1%)   |
| 20  | 1Y    | 0.37         | 0/823   | 0.54        | 0/1099          |
| 20  | 2Y    | 0.33         | 0/823   | 0.51        | 0/1100          |
| 21  | 1Z    | 0.30         | 0/1620  | 0.52        | 0/2200          |
| 21  | 2Z    | 0.30         | 0/1590  | 0.49        | 0/2162          |
| 22  | 10    | 0.35         | 0/616   | 0.56        | 0/821           |
| 22  | 20    | 0.33         | 0/616   | 0.50        | 0/821           |
| 23  | 11    | 0.33         | 0/761   | 0.51        | 0/1013          |
| 23  | 21    | 0.32         | 0/766   | 0.50        | 0/1018          |
| 24  | 12    | 0.30         | 0/590   | 0.51        | 0/781           |
| 24  | 22    | 0.30         | 0/594   | 0.44        | 0/785           |
| 25  | 13    | 0.33         | 0/474   | 0.52        | 0/635           |
| 25  | 23    | 0.30         | 0/469   | 0.49        | 0/630           |
| 26  | 14    | 0.32         | 0/559   | 0.54        | 0/754           |
| 26  | 24    | 0.35         | 0/549   | 0.54        | 0/741           |
| 27  | 15    | 0.40         | 0/473   | 0.65        | 2/639 (0.3%)    |
| 27  | 25    | 0.33         | 0/469   | 0.53        | 0/635           |
| 28  | 16    | 0.33         | 0/460   | 0.56        | 0/613           |
| 28  | 26    | 0.32         | 0/456   | 0.49        | 0/608           |
| 29  | 17    | 0.38         | 0/426   | 0.58        | 0/561           |
| 29  | 27    | 0.31         | 0/426   | 0.50        | 0/561           |
| 30  | 18    | 0.36         | 0/525   | 0.56        | 0/691           |
| 30  | 28    | 0.31         | 0/525   | 0.52        | 0/691           |
| 31  | 19    | 0.37         | 0/310   | 0.53        | 0/407           |
| 31  | 29    | 0.31         | 0/310   | 0.52        | 0/407           |
| 32  | 1a    | 0.37         | 0/35795 | 0.88        | 18/55864 (0.0%) |
| 32  | 2a    | 0.37         | 0/35890 | 0.89        | 32/56012 (0.1%) |
| 33  | 1b    | 0.30         | 0/1876  | 0.50        | 0/2533          |
| 33  | 2b    | 0.33         | 0/1860  | 0.52        | 1/2518 (0.0%)   |
| 34  | 1c    | 0.29         | 0/1582  | 0.47        | 0/2137          |
| 34  | 2c    | 0.30         | 0/1566  | 0.48        | 0/2119          |
| 35  | 1d    | 0.30         | 0/1695  | 0.49        | 0/2274          |
| 35  | 2d    | 0.29         | 0/1698  | 0.46        | 0/2277          |
| 36  | 1e    | 0.31         | 0/1149  | 0.52        | 0/1548          |
| 36  | 2e    | 0.30         | 0/1149  | 0.51        | 0/1548          |
| 37  | 1f    | 0.32         | 0/827   | 0.51        | 0/1120          |
| 37  | 2f    | 0.29         | 0/829   | 0.50        | 0/1123          |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 38  | 1g    | 0.29         | 0/1254   | 0.44        | 0/1683            |
| 38  | 2g    | 0.29         | 0/1248   | 0.43        | 0/1676            |
| 39  | 1h    | 0.28         | 0/1118   | 0.48        | 0/1506            |
| 39  | 2h    | 0.28         | 0/1108   | 0.47        | 0/1494            |
| 40  | 1i    | 0.28         | 0/1005   | 0.50        | 0/1351            |
| 40  | 2i    | 0.30         | 0/985    | 0.47        | 0/1329            |
| 41  | 1j    | 0.30         | 0/732    | 0.49        | 0/993             |
| 41  | 2j    | 0.28         | 0/723    | 0.48        | 0/984             |
| 42  | 1k    | 0.30         | 0/849    | 0.48        | 0/1150            |
| 42  | 2k    | 0.30         | 0/848    | 0.54        | 0/1149            |
| 43  | 1l    | 0.30         | 0/937    | 0.51        | 0/1260            |
| 43  | 2l    | 0.29         | 0/937    | 0.53        | 0/1260            |
| 44  | 1m    | 0.28         | 0/924    | 0.46        | 0/1242            |
| 44  | 2m    | 0.30         | 0/905    | 0.49        | 0/1217            |
| 45  | 1n    | 0.31         | 0/501    | 0.46        | 0/664             |
| 45  | 2n    | 0.31         | 0/501    | 0.47        | 0/664             |
| 46  | 1o    | 0.28         | 0/739    | 0.48        | 0/985             |
| 46  | 2o    | 0.28         | 0/739    | 0.46        | 0/985             |
| 47  | 1p    | 0.30         | 0/697    | 0.53        | 0/939             |
| 47  | 2p    | 0.29         | 0/693    | 0.49        | 0/935             |
| 48  | 1q    | 0.30         | 0/836    | 0.51        | 0/1117            |
| 48  | 2q    | 0.29         | 0/836    | 0.49        | 0/1117            |
| 49  | 1r    | 0.28         | 0/560    | 0.48        | 0/746             |
| 49  | 2r    | 0.28         | 0/560    | 0.47        | 0/746             |
| 50  | 1s    | 0.27         | 0/663    | 0.50        | 0/895             |
| 50  | 2s    | 0.28         | 0/660    | 0.49        | 0/893             |
| 51  | 1t    | 0.27         | 0/734    | 0.45        | 0/969             |
| 51  | 2t    | 0.27         | 0/736    | 0.41        | 0/976             |
| 52  | 1u    | 0.25         | 0/203    | 0.48        | 0/266             |
| 52  | 2u    | 0.32         | 0/203    | 0.51        | 0/266             |
| 53  | 1y    | 0.29         | 0/776    | 0.47        | 0/1048            |
| 53  | 2y    | 0.27         | 0/761    | 0.45        | 0/1030            |
| All | All   | 0.40         | 0/309937 | 0.82        | 149/463223 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 19  | 1X    | 0                   | 1                   |
| 26  | 24    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 33  | 1b    | 0                   | 2                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

The worst 5 of 149 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32  | 2a    | 1003 | G    | N3-C4-C5   | -8.97 | 124.12      | 128.60   |
| 32  | 2a    | 1003 | G    | C8-N9-C4   | -8.85 | 102.86      | 106.40   |
| 1   | 1A    | 537  | G    | O4'-C1'-N9 | 8.36  | 114.89      | 108.20   |
| 1   | 1A    | 354  | A    | C2-N3-C4   | -8.34 | 106.43      | 110.60   |
| 32  | 1a    | 1028 | C    | C2-N3-C4   | 7.73  | 123.77      | 119.90   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 19  | 1X    | 93  | GLU  | Peptide |
| 33  | 1b    | 127 | ILE  | Peptide |
| 33  | 1b    | 231 | GLU  | Peptide |
| 26  | 24    | 18  | CYS  | Peptide |

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 3   | 1D    | 273/276 (99%) | 258 (94%) | 15 (6%) | 0        | 100   100   |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | 2D    | 273/276 (99%) | 258 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 4   | 1E    | 202/206 (98%) | 192 (95%) | 9 (4%)   | 1 (0%)   | 29          | 54  |
| 4   | 2E    | 202/206 (98%) | 192 (95%) | 9 (4%)   | 1 (0%)   | 29          | 54  |
| 5   | 1F    | 201/210 (96%) | 191 (95%) | 9 (4%)   | 1 (0%)   | 29          | 54  |
| 5   | 2F    | 201/210 (96%) | 191 (95%) | 7 (4%)   | 3 (2%)   | 10          | 26  |
| 6   | 1G    | 179/182 (98%) | 163 (91%) | 15 (8%)  | 1 (1%)   | 25          | 50  |
| 6   | 2G    | 179/182 (98%) | 166 (93%) | 10 (6%)  | 3 (2%)   | 9           | 23  |
| 7   | 1H    | 172/180 (96%) | 162 (94%) | 9 (5%)   | 1 (1%)   | 25          | 50  |
| 7   | 2H    | 171/180 (95%) | 152 (89%) | 19 (11%) | 0        | 100         | 100 |
| 8   | 1I    | 145/148 (98%) | 129 (89%) | 15 (10%) | 1 (1%)   | 22          | 46  |
| 8   | 2I    | 144/148 (97%) | 130 (90%) | 12 (8%)  | 2 (1%)   | 11          | 28  |
| 9   | 1N    | 138/140 (99%) | 135 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 130 (94%) | 7 (5%)   | 1 (1%)   | 22          | 46  |
| 10  | 1O    | 120/122 (98%) | 111 (92%) | 8 (7%)   | 1 (1%)   | 19          | 43  |
| 10  | 2O    | 120/122 (98%) | 111 (92%) | 8 (7%)   | 1 (1%)   | 19          | 43  |
| 11  | 1P    | 147/150 (98%) | 138 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 11  | 2P    | 147/150 (98%) | 137 (93%) | 9 (6%)   | 1 (1%)   | 22          | 46  |
| 12  | 1Q    | 139/141 (99%) | 134 (96%) | 4 (3%)   | 1 (1%)   | 22          | 46  |
| 12  | 2Q    | 139/141 (99%) | 131 (94%) | 7 (5%)   | 1 (1%)   | 22          | 46  |
| 13  | 1R    | 116/118 (98%) | 113 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 13  | 2R    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 14  | 1S    | 108/112 (96%) | 99 (92%)  | 8 (7%)   | 1 (1%)   | 17          | 40  |
| 14  | 2S    | 108/112 (96%) | 96 (89%)  | 12 (11%) | 0        | 100         | 100 |
| 15  | 1T    | 129/146 (88%) | 121 (94%) | 7 (5%)   | 1 (1%)   | 19          | 43  |
| 15  | 2T    | 129/146 (88%) | 121 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 16  | 1U    | 114/118 (97%) | 113 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 16  | 2U    | 114/118 (97%) | 109 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 17  | 1V    | 99/101 (98%)  | 97 (98%)  | 1 (1%)   | 1 (1%)   | 15          | 37  |
| 17  | 2V    | 99/101 (98%)  | 93 (94%)  | 5 (5%)   | 1 (1%)   | 15          | 37  |
| 18  | 1W    | 110/113 (97%) | 107 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 107 (97%) | 3 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 19  | 1X    | 93/96 (97%)   | 91 (98%)  | 1 (1%)   | 1 (1%)   | 14          | 34  |
| 19  | 2X    | 93/96 (97%)   | 89 (96%)  | 3 (3%)   | 1 (1%)   | 14          | 34  |
| 20  | 1Y    | 105/110 (96%) | 95 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 20  | 2Y    | 105/110 (96%) | 98 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 21  | 1Z    | 201/206 (98%) | 189 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 21  | 2Z    | 199/206 (97%) | 183 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 22  | 10    | 75/85 (88%)   | 73 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 22  | 20    | 75/85 (88%)   | 72 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 23  | 11    | 95/98 (97%)   | 93 (98%)  | 1 (1%)   | 1 (1%)   | 14          | 34  |
| 23  | 21    | 95/98 (97%)   | 93 (98%)  | 1 (1%)   | 1 (1%)   | 14          | 34  |
| 24  | 12    | 68/72 (94%)   | 67 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 66 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 56 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 25  | 23    | 57/60 (95%)   | 55 (96%)  | 1 (2%)   | 1 (2%)   | 8           | 21  |
| 26  | 14    | 67/71 (94%)   | 52 (78%)  | 12 (18%) | 3 (4%)   | 2           | 5   |
| 26  | 24    | 67/71 (94%)   | 53 (79%)  | 9 (13%)  | 5 (8%)   | 1           | 1   |
| 27  | 15    | 57/60 (95%)   | 57 (100%) | 0        | 0        | 100         | 100 |
| 27  | 25    | 57/60 (95%)   | 55 (96%)  | 1 (2%)   | 1 (2%)   | 8           | 21  |
| 28  | 16    | 51/54 (94%)   | 48 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 47 (92%)  | 4 (8%)   | 0        | 100         | 100 |
| 29  | 17    | 46/49 (94%)   | 46 (100%) | 0        | 0        | 100         | 100 |
| 29  | 27    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 18    | 62/65 (95%)   | 62 (100%) | 0        | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 62 (100%) | 0        | 0        | 100         | 100 |
| 31  | 19    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 34 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 200 (87%) | 20 (9%)  | 9 (4%)   | 3           | 6   |
| 33  | 2b    | 229/256 (90%) | 200 (87%) | 22 (10%) | 7 (3%)   | 4           | 9   |
| 34  | 1c    | 204/239 (85%) | 191 (94%) | 12 (6%)  | 1 (0%)   | 29          | 54  |
| 34  | 2c    | 204/239 (85%) | 172 (84%) | 29 (14%) | 3 (2%)   | 10          | 26  |
| 35  | 1d    | 206/209 (99%) | 192 (93%) | 13 (6%)  | 1 (0%)   | 29          | 54  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 35  | 2d    | 206/209 (99%) | 189 (92%) | 16 (8%)  | 1 (0%)   | 29          | 54  |
| 36  | 1e    | 146/162 (90%) | 141 (97%) | 3 (2%)   | 2 (1%)   | 11          | 28  |
| 36  | 2e    | 146/162 (90%) | 134 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 37  | 1f    | 98/101 (97%)  | 93 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 37  | 2f    | 98/101 (97%)  | 91 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 38  | 1g    | 153/156 (98%) | 145 (95%) | 7 (5%)   | 1 (1%)   | 22          | 46  |
| 38  | 2g    | 153/156 (98%) | 144 (94%) | 7 (5%)   | 2 (1%)   | 12          | 30  |
| 39  | 1h    | 135/138 (98%) | 128 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 39  | 2h    | 135/138 (98%) | 127 (94%) | 7 (5%)   | 1 (1%)   | 22          | 46  |
| 40  | 1i    | 125/128 (98%) | 112 (90%) | 12 (10%) | 1 (1%)   | 19          | 43  |
| 40  | 2i    | 124/128 (97%) | 111 (90%) | 10 (8%)  | 3 (2%)   | 6           | 15  |
| 41  | 1j    | 95/105 (90%)  | 77 (81%)  | 15 (16%) | 3 (3%)   | 4           | 9   |
| 41  | 2j    | 94/105 (90%)  | 80 (85%)  | 12 (13%) | 2 (2%)   | 7           | 18  |
| 42  | 1k    | 112/129 (87%) | 102 (91%) | 9 (8%)   | 1 (1%)   | 17          | 40  |
| 42  | 2k    | 112/129 (87%) | 100 (89%) | 11 (10%) | 1 (1%)   | 17          | 40  |
| 43  | 1l    | 119/132 (90%) | 115 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 43  | 2l    | 119/132 (90%) | 108 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 44  | 1m    | 114/126 (90%) | 104 (91%) | 8 (7%)   | 2 (2%)   | 8           | 21  |
| 44  | 2m    | 112/126 (89%) | 98 (88%)  | 12 (11%) | 2 (2%)   | 8           | 21  |
| 45  | 1n    | 58/61 (95%)   | 56 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 45  | 2n    | 58/61 (95%)   | 53 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 46  | 1o    | 86/89 (97%)   | 82 (95%)  | 1 (1%)   | 3 (4%)   | 3           | 8   |
| 46  | 2o    | 86/89 (97%)   | 83 (96%)  | 2 (2%)   | 1 (1%)   | 13          | 32  |
| 47  | 1p    | 80/88 (91%)   | 72 (90%)  | 7 (9%)   | 1 (1%)   | 12          | 30  |
| 47  | 2p    | 80/88 (91%)   | 68 (85%)  | 11 (14%) | 1 (1%)   | 12          | 30  |
| 48  | 1q    | 97/105 (92%)  | 92 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 48  | 2q    | 97/105 (92%)  | 92 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 49  | 1r    | 66/88 (75%)   | 65 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 49  | 2r    | 66/88 (75%)   | 63 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 50  | 1s    | 81/93 (87%)   | 71 (88%)  | 8 (10%)  | 2 (2%)   | 5           | 14  |
| 50  | 2s    | 81/93 (87%)   | 73 (90%)  | 8 (10%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 51  | 1t    | 94/106 (89%)      | 87 (93%)    | 5 (5%)   | 2 (2%)   | 7           | 18  |
| 51  | 2t    | 96/106 (91%)      | 89 (93%)    | 3 (3%)   | 4 (4%)   | 3           | 5   |
| 52  | 1u    | 21/27 (78%)       | 21 (100%)   | 0        | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)       | 16 (76%)    | 4 (19%)  | 1 (5%)   | 2           | 4   |
| 53  | 1y    | 95/113 (84%)      | 90 (95%)    | 5 (5%)   | 0        | 100         | 100 |
| 53  | 2y    | 94/113 (83%)      | 88 (94%)    | 6 (6%)   | 0        | 100         | 100 |
| All | All   | 11629/12354 (94%) | 10827 (93%) | 706 (6%) | 96 (1%)  | 19          | 43  |

5 of 96 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | 14    | 47  | GLN  |
| 26  | 14    | 55  | ARG  |
| 33  | 1b    | 21  | ARG  |
| 4   | 2E    | 51  | PHE  |
| 6   | 2G    | 78  | SER  |

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | 1D    | 214/218 (98%) | 195 (91%) | 19 (9%)  | 9           | 22 |
| 3   | 2D    | 215/218 (99%) | 197 (92%) | 18 (8%)  | 11          | 25 |
| 4   | 1E    | 164/166 (99%) | 151 (92%) | 13 (8%)  | 12          | 28 |
| 4   | 2E    | 164/166 (99%) | 154 (94%) | 10 (6%)  | 18          | 41 |
| 5   | 1F    | 160/166 (96%) | 145 (91%) | 15 (9%)  | 8           | 20 |
| 5   | 2F    | 159/166 (96%) | 148 (93%) | 11 (7%)  | 15          | 35 |
| 6   | 1G    | 144/156 (92%) | 132 (92%) | 12 (8%)  | 11          | 25 |
| 6   | 2G    | 142/156 (91%) | 129 (91%) | 13 (9%)  | 9           | 21 |
| 7   | 1H    | 144/148 (97%) | 138 (96%) | 6 (4%)   | 30          | 58 |
| 7   | 2H    | 143/148 (97%) | 137 (96%) | 6 (4%)   | 30          | 58 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 8   | 1I    | 111/124 (90%)  | 104 (94%) | 7 (6%)   | 18          | 40 |
| 8   | 2I    | 108/124 (87%)  | 103 (95%) | 5 (5%)   | 27          | 54 |
| 9   | 1N    | 119/119 (100%) | 112 (94%) | 7 (6%)   | 19          | 43 |
| 9   | 2N    | 118/119 (99%)  | 112 (95%) | 6 (5%)   | 24          | 50 |
| 10  | 1O    | 100/100 (100%) | 96 (96%)  | 4 (4%)   | 31          | 60 |
| 10  | 2O    | 100/100 (100%) | 96 (96%)  | 4 (4%)   | 31          | 60 |
| 11  | 1P    | 115/116 (99%)  | 112 (97%) | 3 (3%)   | 46          | 75 |
| 11  | 2P    | 115/116 (99%)  | 110 (96%) | 5 (4%)   | 29          | 57 |
| 12  | 1Q    | 111/111 (100%) | 104 (94%) | 7 (6%)   | 18          | 40 |
| 12  | 2Q    | 111/111 (100%) | 107 (96%) | 4 (4%)   | 35          | 64 |
| 13  | 1R    | 101/101 (100%) | 91 (90%)  | 10 (10%) | 8           | 18 |
| 13  | 2R    | 101/101 (100%) | 89 (88%)  | 12 (12%) | 5           | 12 |
| 14  | 1S    | 87/88 (99%)    | 80 (92%)  | 7 (8%)   | 12          | 27 |
| 14  | 2S    | 85/88 (97%)    | 79 (93%)  | 6 (7%)   | 14          | 34 |
| 15  | 1T    | 115/127 (91%)  | 110 (96%) | 5 (4%)   | 29          | 57 |
| 15  | 2T    | 113/127 (89%)  | 107 (95%) | 6 (5%)   | 22          | 48 |
| 16  | 1U    | 93/94 (99%)    | 88 (95%)  | 5 (5%)   | 22          | 47 |
| 16  | 2U    | 93/94 (99%)    | 90 (97%)  | 3 (3%)   | 39          | 68 |
| 17  | 1V    | 81/82 (99%)    | 73 (90%)  | 8 (10%)  | 8           | 18 |
| 17  | 2V    | 80/82 (98%)    | 76 (95%)  | 4 (5%)   | 24          | 51 |
| 18  | 1W    | 90/92 (98%)    | 81 (90%)  | 9 (10%)  | 7           | 18 |
| 18  | 2W    | 90/92 (98%)    | 82 (91%)  | 8 (9%)   | 9           | 22 |
| 19  | 1X    | 77/78 (99%)    | 73 (95%)  | 4 (5%)   | 23          | 49 |
| 19  | 2X    | 77/78 (99%)    | 73 (95%)  | 4 (5%)   | 23          | 49 |
| 20  | 1Y    | 86/91 (94%)    | 80 (93%)  | 6 (7%)   | 15          | 35 |
| 20  | 2Y    | 86/91 (94%)    | 84 (98%)  | 2 (2%)   | 50          | 78 |
| 21  | 1Z    | 169/179 (94%)  | 154 (91%) | 15 (9%)  | 9           | 22 |
| 21  | 2Z    | 165/179 (92%)  | 158 (96%) | 7 (4%)   | 30          | 58 |
| 22  | 10    | 61/67 (91%)    | 57 (93%)  | 4 (7%)   | 16          | 38 |
| 22  | 20    | 61/67 (91%)    | 59 (97%)  | 2 (3%)   | 38          | 67 |
| 23  | 11    | 79/83 (95%)    | 76 (96%)  | 3 (4%)   | 33          | 62 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 23  | 21    | 81/83 (98%)   | 78 (96%)  | 3 (4%)   | 34          | 63  |
| 24  | 12    | 65/67 (97%)   | 64 (98%)  | 1 (2%)   | 65          | 86  |
| 24  | 22    | 66/67 (98%)   | 65 (98%)  | 1 (2%)   | 65          | 86  |
| 25  | 13    | 51/52 (98%)   | 46 (90%)  | 5 (10%)  | 8           | 18  |
| 25  | 23    | 50/52 (96%)   | 48 (96%)  | 2 (4%)   | 31          | 60  |
| 26  | 14    | 58/63 (92%)   | 55 (95%)  | 3 (5%)   | 23          | 49  |
| 26  | 24    | 54/63 (86%)   | 54 (100%) | 0        | 100         | 100 |
| 27  | 15    | 51/52 (98%)   | 45 (88%)  | 6 (12%)  | 5           | 12  |
| 27  | 25    | 50/52 (96%)   | 47 (94%)  | 3 (6%)   | 19          | 42  |
| 28  | 16    | 51/52 (98%)   | 46 (90%)  | 5 (10%)  | 8           | 18  |
| 28  | 26    | 50/52 (96%)   | 46 (92%)  | 4 (8%)   | 12          | 27  |
| 29  | 17    | 41/42 (98%)   | 36 (88%)  | 5 (12%)  | 5           | 11  |
| 29  | 27    | 41/42 (98%)   | 41 (100%) | 0        | 100         | 100 |
| 30  | 18    | 54/55 (98%)   | 50 (93%)  | 4 (7%)   | 13          | 32  |
| 30  | 28    | 54/55 (98%)   | 49 (91%)  | 5 (9%)   | 9           | 21  |
| 31  | 19    | 34/34 (100%)  | 32 (94%)  | 2 (6%)   | 19          | 43  |
| 31  | 29    | 34/34 (100%)  | 33 (97%)  | 1 (3%)   | 42          | 71  |
| 33  | 1b    | 191/220 (87%) | 183 (96%) | 8 (4%)   | 30          | 58  |
| 33  | 2b    | 187/220 (85%) | 180 (96%) | 7 (4%)   | 34          | 63  |
| 34  | 1c    | 144/188 (77%) | 139 (96%) | 5 (4%)   | 36          | 65  |
| 34  | 2c    | 140/188 (74%) | 134 (96%) | 6 (4%)   | 29          | 57  |
| 35  | 1d    | 171/181 (94%) | 162 (95%) | 9 (5%)   | 22          | 48  |
| 35  | 2d    | 172/181 (95%) | 166 (96%) | 6 (4%)   | 36          | 65  |
| 36  | 1e    | 114/123 (93%) | 110 (96%) | 4 (4%)   | 36          | 65  |
| 36  | 2e    | 114/123 (93%) | 108 (95%) | 6 (5%)   | 22          | 48  |
| 37  | 1f    | 85/90 (94%)   | 82 (96%)  | 3 (4%)   | 36          | 65  |
| 37  | 2f    | 85/90 (94%)   | 82 (96%)  | 3 (4%)   | 36          | 65  |
| 38  | 1g    | 120/127 (94%) | 117 (98%) | 3 (2%)   | 47          | 76  |
| 38  | 2g    | 119/127 (94%) | 113 (95%) | 6 (5%)   | 24          | 51  |
| 39  | 1h    | 116/119 (98%) | 114 (98%) | 2 (2%)   | 60          | 84  |
| 39  | 2h    | 114/119 (96%) | 109 (96%) | 5 (4%)   | 28          | 56  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 40  | 1i    | 91/99 (92%)      | 91 (100%)  | 0        | 100         | 100 |
| 40  | 2i    | 88/99 (89%)      | 85 (97%)   | 3 (3%)   | 37          | 66  |
| 41  | 1j    | 68/92 (74%)      | 66 (97%)   | 2 (3%)   | 42          | 71  |
| 41  | 2j    | 68/92 (74%)      | 67 (98%)   | 1 (2%)   | 65          | 86  |
| 42  | 1k    | 83/99 (84%)      | 80 (96%)   | 3 (4%)   | 35          | 64  |
| 42  | 2k    | 83/99 (84%)      | 79 (95%)   | 4 (5%)   | 25          | 53  |
| 43  | 1l    | 96/108 (89%)     | 92 (96%)   | 4 (4%)   | 30          | 58  |
| 43  | 2l    | 96/108 (89%)     | 94 (98%)   | 2 (2%)   | 53          | 80  |
| 44  | 1m    | 90/101 (89%)     | 86 (96%)   | 4 (4%)   | 28          | 56  |
| 44  | 2m    | 87/101 (86%)     | 84 (97%)   | 3 (3%)   | 37          | 66  |
| 45  | 1n    | 49/50 (98%)      | 48 (98%)   | 1 (2%)   | 55          | 81  |
| 45  | 2n    | 49/50 (98%)      | 49 (100%)  | 0        | 100         | 100 |
| 46  | 1o    | 78/80 (98%)      | 74 (95%)   | 4 (5%)   | 24          | 50  |
| 46  | 2o    | 78/80 (98%)      | 77 (99%)   | 1 (1%)   | 69          | 87  |
| 47  | 1p    | 69/74 (93%)      | 65 (94%)   | 4 (6%)   | 20          | 43  |
| 47  | 2p    | 68/74 (92%)      | 62 (91%)   | 6 (9%)   | 10          | 23  |
| 48  | 1q    | 94/97 (97%)      | 89 (95%)   | 5 (5%)   | 22          | 48  |
| 48  | 2q    | 94/97 (97%)      | 89 (95%)   | 5 (5%)   | 22          | 48  |
| 49  | 1r    | 59/77 (77%)      | 58 (98%)   | 1 (2%)   | 60          | 84  |
| 49  | 2r    | 59/77 (77%)      | 53 (90%)   | 6 (10%)  | 7           | 17  |
| 50  | 1s    | 68/80 (85%)      | 67 (98%)   | 1 (2%)   | 65          | 86  |
| 50  | 2s    | 67/80 (84%)      | 65 (97%)   | 2 (3%)   | 41          | 70  |
| 51  | 1t    | 71/82 (87%)      | 67 (94%)   | 4 (6%)   | 21          | 45  |
| 51  | 2t    | 70/82 (85%)      | 65 (93%)   | 5 (7%)   | 14          | 34  |
| 52  | 1u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)   | 21          | 45  |
| 52  | 2u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)   | 21          | 45  |
| 53  | 1y    | 82/98 (84%)      | 78 (95%)   | 4 (5%)   | 25          | 52  |
| 53  | 2y    | 79/98 (81%)      | 74 (94%)   | 5 (6%)   | 18          | 40  |
| All | All   | 9524/10260 (93%) | 9014 (95%) | 510 (5%) | 22          | 47  |

5 of 510 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | 1g    | 115 | ARG  |
| 35  | 2d    | 135 | LEU  |
| 3   | 2D    | 229 | VAL  |
| 34  | 2c    | 68  | VAL  |
| 42  | 2k    | 116 | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 2F    | 133 | ASN  |
| 25  | 23    | 32  | GLN  |
| 50  | 2s    | 69  | HIS  |
| 6   | 2G    | 79  | ASN  |
| 12  | 2Q    | 141 | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2862/2915 (98%) | 421 (14%)         | 29 (1%)         |
| 1   | 2A    | 2855/2915 (97%) | 492 (17%)         | 36 (1%)         |
| 2   | 1B    | 119/121 (98%)   | 11 (9%)           | 0               |
| 2   | 2B    | 119/121 (98%)   | 18 (15%)          | 0               |
| 32  | 1a    | 1494/1521 (98%) | 233 (15%)         | 0               |
| 32  | 2a    | 1498/1521 (98%) | 261 (17%)         | 0               |
| All | All   | 8947/9114 (98%) | 1436 (16%)        | 65 (0%)         |

5 of 1436 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 14  | A    |
| 1   | 1A    | 15  | G    |
| 1   | 1A    | 34  | C    |
| 1   | 1A    | 45  | C    |

5 of 65 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2288 | A    |
| 1   | 2A    | 2321 | G    |
| 1   | 1A    | 2418 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2250 | G    |
| 1   | 2A    | 2406 | U    |

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |       | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 32  | 5MC  | 2a    | 1404 | 32    | 18,22,23     | 0.95 | 2 (11%)     | 26,32,35    | 1.24 | 4 (15%)     |
| 32  | 7MG  | 1a    | 527  | 32,54 | 22,26,27     | 1.43 | 3 (13%)     | 29,39,42    | 2.34 | 7 (24%)     |
| 1   | PSU  | 2A    | 1911 | 1     | 18,21,22     | 1.37 | 2 (11%)     | 22,30,33    | 1.91 | 3 (13%)     |
| 1   | 5MU  | 1A    | 1961 | 54,1  | 19,22,23     | 1.45 | 5 (26%)     | 28,32,35    | 2.20 | 6 (21%)     |
| 1   | 5MC  | 2A    | 1942 | 1     | 18,22,23     | 0.97 | 2 (11%)     | 26,32,35    | 1.22 | 2 (7%)      |
| 1   | 2MA  | 1A    | 2515 | 54,1  | 17,25,26     | 1.01 | 1 (5%)      | 17,37,40    | 1.05 | 2 (11%)     |
| 32  | MA6  | 1a    | 1519 | 32    | 19,26,27     | 1.02 | 1 (5%)      | 18,38,41    | 1.54 | 4 (22%)     |
| 1   | PSU  | 2A    | 2605 | 1     | 18,21,22     | 1.40 | 3 (16%)     | 22,30,33    | 1.82 | 4 (18%)     |
| 32  | 7MG  | 2a    | 527  | 32,54 | 22,26,27     | 1.35 | 4 (18%)     | 29,39,42    | 2.46 | 5 (17%)     |
| 32  | 4OC  | 1a    | 1402 | 32    | 20,23,24     | 0.72 | 0           | 26,32,35    | 0.97 | 2 (7%)      |
| 32  | UR3  | 1a    | 1498 | 32    | 19,22,23     | 0.96 | 1 (5%)      | 26,32,35    | 1.54 | 2 (7%)      |
| 1   | 4OC  | 2A    | 1920 | 1     | 19,22,24     | 0.82 | 0           | 26,31,35    | 0.92 | 1 (3%)      |
| 32  | PSU  | 2a    | 516  | 32,54 | 18,21,22     | 1.31 | 2 (11%)     | 22,30,33    | 1.92 | 5 (22%)     |
| 32  | 2MG  | 2a    | 1207 | 32    | 18,26,27     | 0.85 | 0           | 16,38,41    | 1.08 | 1 (6%)      |
| 32  | 5MC  | 2a    | 967  | 32    | 18,22,23     | 1.01 | 2 (11%)     | 26,32,35    | 1.19 | 3 (11%)     |
| 32  | M2G  | 1a    | 966  | 32    | 20,27,28     | 1.36 | 3 (15%)     | 22,40,43    | 1.06 | 2 (9%)      |
| 43  | 0TD  | 2l    | 92   | 43    | 7,9,10       | 4.67 | 1 (14%)     | 6,11,13     | 4.28 | 3 (50%)     |
| 1   | 2MA  | 2A    | 2503 | 54,1  | 17,25,26     | 0.96 | 0           | 17,37,40    | 1.09 | 2 (11%)     |
| 32  | 5MC  | 1a    | 1407 | 32    | 18,22,23     | 0.95 | 1 (5%)      | 26,32,35    | 1.20 | 3 (11%)     |
| 32  | MA6  | 2a    | 1518 | 32    | 19,26,27     | 1.05 | 1 (5%)      | 18,38,41    | 1.67 | 4 (22%)     |
| 1   | 5MC  | 1A    | 1964 | 54,1  | 18,22,23     | 0.97 | 2 (11%)     | 26,32,35    | 1.13 | 2 (7%)      |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | 2MG  | 1a    | 1207 | 32    | 18,26,27     | 1.03 | 1 (5%)   | 16,38,41    | 1.51 | 5 (31%)  |
| 1   | 5MU  | 2A    | 1915 | 1     | 19,22,23     | 1.43 | 4 (21%)  | 28,32,35    | 2.18 | 8 (28%)  |
| 1   | 5MC  | 1A    | 1984 | 54,1  | 18,22,23     | 1.01 | 2 (11%)  | 26,32,35    | 1.20 | 4 (15%)  |
| 32  | PSU  | 1a    | 516  | 32,54 | 18,21,22     | 1.38 | 2 (11%)  | 22,30,33    | 1.79 | 4 (18%)  |
| 1   | 5MU  | 1A    | 1937 | 1     | 19,22,23     | 1.44 | 4 (21%)  | 28,32,35    | 2.18 | 8 (28%)  |
| 1   | 5MU  | 2A    | 1939 | 1     | 19,22,23     | 1.45 | 5 (26%)  | 28,32,35    | 2.28 | 6 (21%)  |
| 32  | 4OC  | 2a    | 1402 | 32    | 20,23,24     | 0.77 | 0        | 26,32,35    | 1.11 | 1 (3%)   |
| 1   | 4OC  | 1A    | 1942 | 1     | 19,22,24     | 0.82 | 0        | 26,31,35    | 0.87 | 1 (3%)   |
| 1   | OMG  | 1A    | 2263 | 54,1  | 18,26,27     | 1.05 | 1 (5%)   | 19,38,41    | 1.12 | 2 (10%)  |
| 1   | 2MU  | 2A    | 2552 | 54,1  | 19,22,24     | 1.22 | 3 (15%)  | 26,31,36    | 1.91 | 6 (23%)  |
| 1   | PSU  | 1A    | 2617 | 54,1  | 18,21,22     | 1.38 | 3 (16%)  | 22,30,33    | 1.79 | 4 (18%)  |
| 32  | MA6  | 2a    | 1519 | 32    | 19,26,27     | 0.97 | 1 (5%)   | 18,38,41    | 1.84 | 5 (27%)  |
| 32  | M2G  | 2a    | 966  | 32    | 20,27,28     | 1.55 | 4 (20%)  | 22,40,43    | 0.81 | 1 (4%)   |
| 32  | 5MC  | 1a    | 967  | 32    | 18,22,23     | 1.01 | 2 (11%)  | 26,32,35    | 1.13 | 2 (7%)   |
| 1   | PSU  | 1A    | 1933 | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 2.01 | 4 (18%)  |
| 1   | PSU  | 2A    | 1917 | 1     | 18,21,22     | 1.32 | 2 (11%)  | 22,30,33    | 1.94 | 3 (13%)  |
| 32  | 5MC  | 2a    | 1407 | 32    | 18,22,23     | 0.98 | 2 (11%)  | 26,32,35    | 1.18 | 3 (11%)  |
| 1   | 2MU  | 1A    | 2564 | 54,1  | 19,22,24     | 1.32 | 4 (21%)  | 26,31,36    | 1.79 | 6 (23%)  |
| 1   | 5MC  | 2A    | 1962 | 54,1  | 18,22,23     | 0.94 | 2 (11%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 1   | PSU  | 1A    | 1939 | 1     | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.74 | 4 (18%)  |
| 32  | 5MC  | 1a    | 1404 | 32    | 18,22,23     | 0.92 | 2 (11%)  | 26,32,35    | 1.14 | 3 (11%)  |
| 32  | 5MC  | 2a    | 1400 | 32    | 18,22,23     | 0.95 | 2 (11%)  | 26,32,35    | 1.23 | 2 (7%)   |
| 32  | MA6  | 1a    | 1518 | 32    | 19,26,27     | 0.96 | 1 (5%)   | 18,38,41    | 1.66 | 5 (27%)  |
| 1   | OMG  | 2A    | 2251 | 54,1  | 18,26,27     | 0.87 | 1 (5%)   | 19,38,41    | 1.19 | 3 (15%)  |
| 32  | UR3  | 2a    | 1498 | 32,54 | 19,22,23     | 0.95 | 1 (5%)   | 26,32,35    | 1.48 | 2 (7%)   |
| 32  | 5MC  | 1a    | 1400 | 32    | 18,22,23     | 0.98 | 2 (11%)  | 26,32,35    | 1.19 | 3 (11%)  |
| 43  | 0TD  | 1l    | 92   | 43    | 7,9,10       | 4.80 | 1 (14%)  | 6,11,13     | 3.20 | 3 (50%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 32  | 5MC  | 2a    | 1404 | 32    | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 7MG  | 1a    | 527  | 32,54 | -       | 0/7/37/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 1   | PSU  | 2A    | 1911 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1961 | 54,1  | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1942 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 2MA  | 1A    | 2515 | 54,1  | -       | 2/3/25/26 | 0/3/3/3 |
| 32  | MA6  | 1a    | 1519 | 32    | -       | 3/7/29/30 | 0/3/3/3 |
| 1   | PSU  | 2A    | 2605 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 7MG  | 2a    | 527  | 32,54 | -       | 0/7/37/38 | 0/3/3/3 |
| 32  | 4OC  | 1a    | 1402 | 32    | -       | 2/9/29/30 | 0/2/2/2 |
| 32  | UR3  | 1a    | 1498 | 32    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 4OC  | 2A    | 1920 | 1     | -       | 0/9/27/30 | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 32,54 | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 2MG  | 2a    | 1207 | 32    | -       | 0/5/27/28 | 0/3/3/3 |
| 32  | 5MC  | 2a    | 967  | 32    | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | M2G  | 1a    | 966  | 32    | -       | 0/7/29/30 | 0/3/3/3 |
| 43  | 0TD  | 2l    | 92   | 43    | -       | 1/7/12/14 | -       |
| 1   | 2MA  | 2A    | 2503 | 54,1  | -       | 1/3/25/26 | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1407 | 32    | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | MA6  | 2a    | 1518 | 32    | -       | 2/7/29/30 | 0/3/3/3 |
| 1   | 5MC  | 1A    | 1964 | 54,1  | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 2MG  | 1a    | 1207 | 32    | -       | 2/5/27/28 | 0/3/3/3 |
| 1   | 5MU  | 2A    | 1915 | 1     | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1984 | 54,1  | -       | 2/7/25/26 | 0/2/2/2 |
| 32  | PSU  | 1a    | 516  | 32,54 | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1937 | 1     | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 4OC  | 2a    | 1402 | 32    | -       | 2/9/29/30 | 0/2/2/2 |
| 1   | 4OC  | 1A    | 1942 | 1     | -       | 1/9/27/30 | 0/2/2/2 |
| 1   | OMG  | 1A    | 2263 | 54,1  | -       | 1/5/27/28 | 0/3/3/3 |
| 1   | 2MU  | 2A    | 2552 | 54,1  | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | PSU  | 1A    | 2617 | 54,1  | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | MA6  | 2a    | 1519 | 32    | -       | 4/7/29/30 | 0/3/3/3 |
| 32  | M2G  | 2a    | 966  | 32    | -       | 0/7/29/30 | 0/3/3/3 |
| 32  | 5MC  | 1a    | 967  | 32    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 1A    | 1933 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 2A    | 1917 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1407 | 32    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 2MU  | 1A    | 2564 | 54,1  | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 54,1  | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 1A    | 1939 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1404 | 32    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 32  | 5MC  | 2a    | 1400 | 32    | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | MA6  | 1a    | 1518 | 32    | -       | 3/7/29/30 | 0/3/3/3 |
| 1   | OMG  | 2A    | 2251 | 54,1  | -       | 0/5/27/28 | 0/3/3/3 |
| 32  | UR3  | 2a    | 1498 | 32,54 | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1400 | 32    | -       | 1/7/25/26 | 0/2/2/2 |
| 43  | 0TD  | 1l    | 92   | 43    | -       | 3/7/12/14 | -       |

The worst 5 of 92 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 43  | 1l    | 92  | 0TD  | CB-SB | -12.29 | 1.69        | 1.82     |
| 43  | 2l    | 92  | 0TD  | CB-SB | -12.04 | 1.70        | 1.82     |
| 32  | 2a    | 966 | M2G  | C2-N3 | 4.91   | 1.36        | 1.30     |
| 32  | 1a    | 966 | M2G  | C2-N3 | 4.02   | 1.35        | 1.30     |
| 32  | 1a    | 527 | 7MG  | C4-N9 | -3.94  | 1.33        | 1.37     |

The worst 5 of 167 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB | -9.79 | 84.73       | 102.44   |
| 32  | 2a    | 527  | 7MG  | N9-C4-N3  | 8.32  | 137.92      | 125.47   |
| 32  | 1a    | 527  | 7MG  | N9-C4-N3  | 8.04  | 137.50      | 125.47   |
| 32  | 1a    | 1498 | UR3  | C4-N3-C2  | -6.40 | 118.53      | 124.56   |
| 1   | 1A    | 1933 | PSU  | N1-C2-N3  | 6.37  | 122.35      | 115.13   |

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 1   | 1A    | 1937 | 5MU  | O4'-C1'-N1-C2 |
| 1   | 1A    | 1937 | 5MU  | O4'-C1'-N1-C6 |
| 32  | 1a    | 1207 | 2MG  | N1-C2-N2-CM2  |
| 32  | 1a    | 1207 | 2MG  | N3-C2-N2-CM2  |
| 32  | 1a    | 1518 | MA6  | C5-C6-N6-C9   |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2389 ligands modelled in this entry, 2376 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | EZP  | 1A    | 3987 | -    | 21,26,26     | 2.81 | 3 (14%)  | 26,35,35    | 1.72 | 4 (15%)  |
| 60  | SF4  | 1d    | 302  | 35   | 0,12,12      | -    | -        | -           | -    | -        |
| 60  | SF4  | 2d    | 501  | 35   | 0,12,12      | -    | -        | -           | -    | -        |
| 57  | MPD  | 1a    | 1854 | -    | 7,7,7        | 0.38 | 0        | 9,10,10     | 0.38 | 0        |
| 56  | EZP  | 2A    | 3709 | -    | 21,26,26     | 3.58 | 3 (14%)  | 26,35,35    | 0.92 | 1 (3%)   |
| 57  | MPD  | 1T    | 204  | -    | 7,7,7        | 0.32 | 0        | 9,10,10     | 0.36 | 0        |
| 57  | MPD  | 1A    | 3988 | -    | 7,7,7        | 0.27 | 0        | 9,10,10     | 0.28 | 0        |
| 58  | ARG  | 1F    | 314  | -    | 10,11,11     | 0.70 | 0        | 11,13,13    | 1.03 | 2 (18%)  |
| 57  | MPD  | 2A    | 3711 | -    | 7,7,7        | 0.30 | 0        | 9,10,10     | 0.30 | 0        |
| 57  | MPD  | 18    | 102  | -    | 7,7,7        | 0.27 | 0        | 9,10,10     | 0.38 | 0        |
| 57  | MPD  | 2A    | 3710 | -    | 7,7,7        | 0.39 | 0        | 9,10,10     | 0.30 | 0        |
| 58  | ARG  | 1B    | 228  | 54   | 10,11,11     | 0.74 | 1 (10%)  | 11,13,13    | 1.16 | 2 (18%)  |
| 57  | MPD  | 2B    | 3020 | -    | 7,7,7        | 0.30 | 0        | 9,10,10     | 0.30 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 56  | EZP  | 1A    | 3987 | -    | -       | 7/24/26/26 | 0/2/2/2 |
| 60  | SF4  | 1d    | 302  | 35   | -       | -          | 0/6/5/5 |
| 60  | SF4  | 2d    | 501  | 35   | -       | -          | 0/6/5/5 |
| 57  | MPD  | 1a    | 1854 | -    | -       | 2/5/5/5    | -       |
| 56  | EZP  | 2A    | 3709 | -    | -       | 7/24/26/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 57  | MPD  | 1T    | 204  | -    | -       | 1/5/5/5    | -     |
| 57  | MPD  | 1A    | 3988 | -    | -       | 2/5/5/5    | -     |
| 58  | ARG  | 1F    | 314  | -    | -       | 1/11/11/11 | -     |
| 57  | MPD  | 2A    | 3711 | -    | -       | 3/5/5/5    | -     |
| 57  | MPD  | 18    | 102  | -    | -       | 1/5/5/5    | -     |
| 57  | MPD  | 2A    | 3710 | -    | -       | 0/5/5/5    | -     |
| 58  | ARG  | 1B    | 228  | 54   | -       | 4/11/11/11 | -     |
| 57  | MPD  | 2B    | 3020 | -    | -       | 3/5/5/5    | -     |

The worst 5 of 7 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 56  | 2A    | 3709 | EZP  | OAC-NAY | 13.50 | 1.45        | 1.22     |
| 56  | 1A    | 3987 | EZP  | OAC-NAY | 9.18  | 1.38        | 1.22     |
| 56  | 2A    | 3709 | EZP  | CAT-CAW | -8.10 | 1.39        | 1.51     |
| 56  | 1A    | 3987 | EZP  | CAT-CAW | -7.46 | 1.40        | 1.51     |
| 56  | 1A    | 3987 | EZP  | CAU-NAY | -4.60 | 1.34        | 1.45     |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56  | 1A    | 3987 | EZP  | CAT-CAW-CAX | 4.98  | 120.42      | 111.64   |
| 56  | 1A    | 3987 | EZP  | CAW-CAX-NAP | 4.35  | 118.30      | 110.05   |
| 58  | 1B    | 228  | ARG  | OXT-C-O     | -2.68 | 118.01      | 124.09   |
| 56  | 1A    | 3987 | EZP  | CAI-CAU-NAY | 2.44  | 121.22      | 119.38   |
| 58  | 1F    | 314  | ARG  | OXT-C-O     | -2.43 | 118.57      | 124.09   |

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

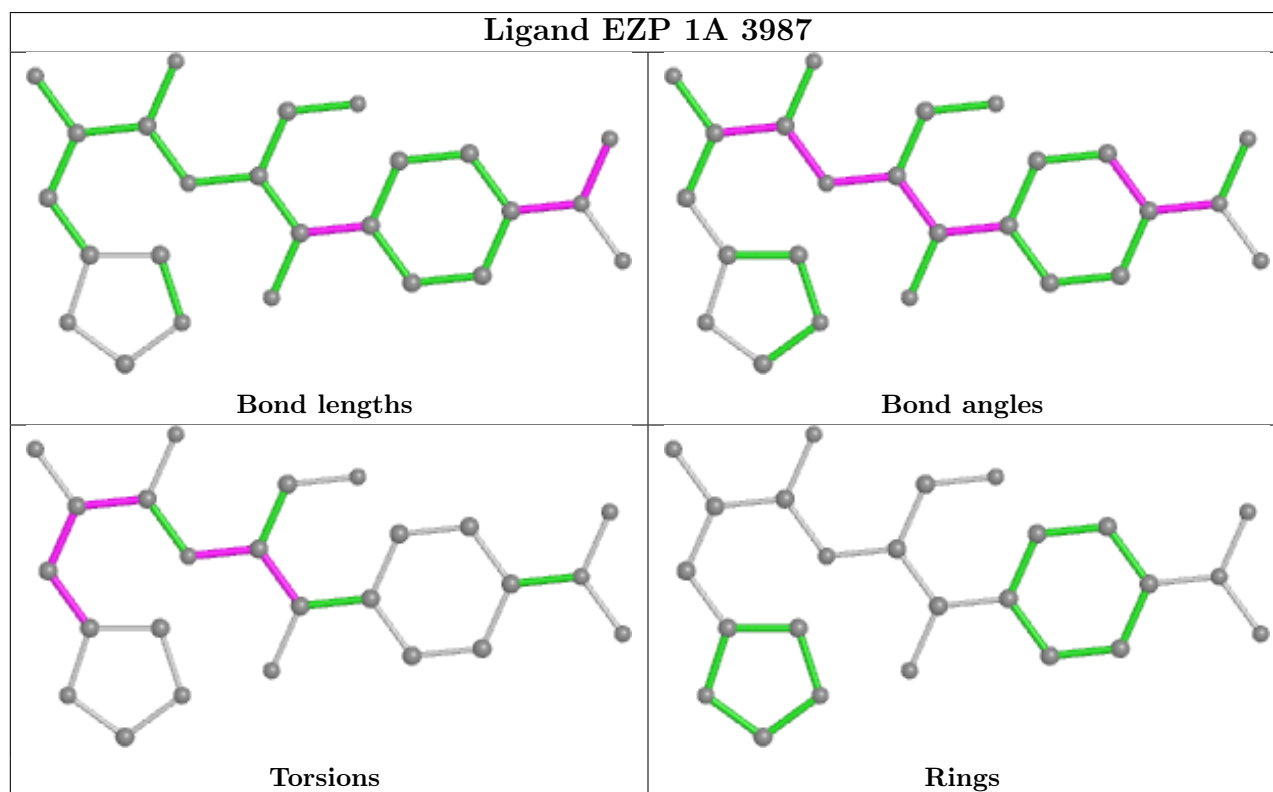
| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 56  | 1A    | 3987 | EZP  | NAP-C-CA-CB |
| 56  | 1A    | 3987 | EZP  | O-C-CA-CB   |
| 56  | 1A    | 3987 | EZP  | C-CA-CB-CG  |
| 56  | 2A    | 3709 | EZP  | NAP-C-CA-N  |
| 56  | 2A    | 3709 | EZP  | NAP-C-CA-CB |

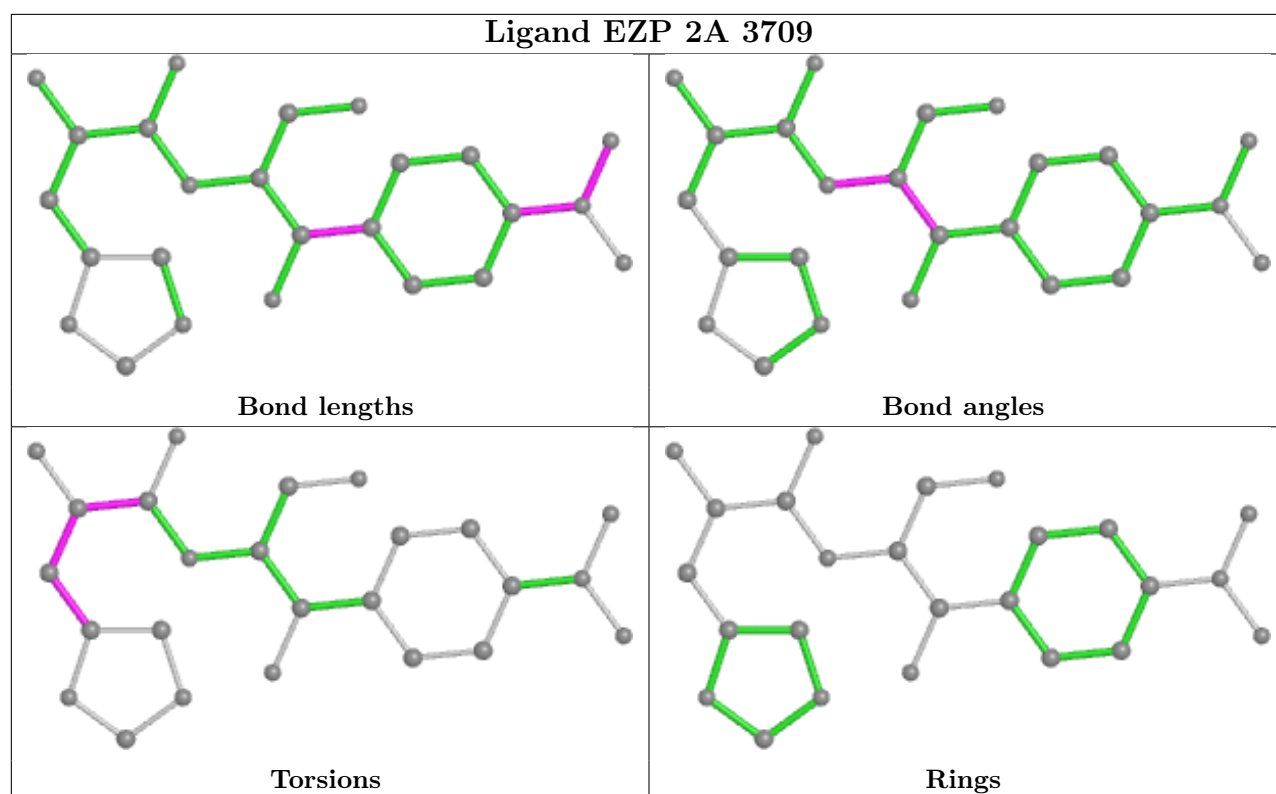
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | 1A    | 2861/2915 (98%) | 0.42   | 57 (1%) 65 67 | 15, 31, 89, 105       | 0     |
| 1   | 2A    | 2856/2915 (97%) | 0.28   | 65 (2%) 60 62 | 27, 50, 92, 103       | 0     |
| 2   | 1B    | 120/121 (99%)   | 0.05   | 0 100 100     | 24, 44, 58, 80        | 0     |
| 2   | 2B    | 120/121 (99%)   | -0.06  | 0 100 100     | 52, 74, 83, 90        | 0     |
| 3   | 1D    | 275/276 (99%)   | 0.60   | 3 (1%) 80 82  | 17, 32, 46, 65        | 0     |
| 3   | 2D    | 275/276 (99%)   | 0.69   | 13 (4%) 31 30 | 26, 44, 56, 76        | 0     |
| 4   | 1E    | 204/206 (99%)   | 0.51   | 2 (0%) 82 83  | 16, 34, 55, 70        | 0     |
| 4   | 2E    | 204/206 (99%)   | 0.59   | 3 (1%) 73 76  | 29, 50, 66, 79        | 0     |
| 5   | 1F    | 203/210 (96%)   | 0.37   | 0 100 100     | 16, 35, 60, 83        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.39   | 3 (1%) 73 76  | 29, 60, 72, 85        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.16   | 2 (1%) 80 82  | 39, 56, 72, 80        | 0     |
| 6   | 2G    | 181/182 (99%)   | 0.59   | 13 (7%) 15 13 | 68, 77, 85, 89        | 0     |
| 7   | 1H    | 174/180 (96%)   | 0.29   | 1 (0%) 89 91  | 32, 46, 59, 64        | 0     |
| 7   | 2H    | 173/180 (96%)   | 0.72   | 20 (11%) 4 3  | 62, 75, 82, 86        | 0     |
| 8   | 1I    | 147/148 (99%)   | 0.15   | 3 (2%) 65 67  | 34, 66, 76, 83        | 0     |
| 8   | 2I    | 146/148 (98%)   | 0.49   | 15 (10%) 6 5  | 51, 69, 81, 84        | 0     |
| 9   | 1N    | 140/140 (100%)  | 0.41   | 0 100 100     | 22, 32, 53, 67        | 0     |
| 9   | 2N    | 140/140 (100%)  | 0.41   | 1 (0%) 87 89  | 43, 57, 71, 76        | 0     |
| 10  | 1O    | 122/122 (100%)  | 0.47   | 0 100 100     | 23, 34, 50, 58        | 0     |
| 10  | 2O    | 122/122 (100%)  | 0.58   | 5 (4%) 37 36  | 38, 51, 61, 69        | 0     |
| 11  | 1P    | 149/150 (99%)   | 0.36   | 1 (0%) 87 89  | 15, 38, 58, 71        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.66   | 7 (4%) 31 30  | 32, 59, 77, 80        | 0     |
| 12  | 1Q    | 141/141 (100%)  | 0.44   | 0 100 100     | 21, 35, 46, 62        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 0.66   | 7 (4%) 28 27  | 40, 57, 67, 76        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | 0.50   | 0 100 100    | 21, 29, 44, 50        | 0     |
| 13  | 2R    | 118/118 (100%) | 0.45   | 2 (1%) 70 72 | 31, 44, 55, 65        | 0     |
| 14  | 1S    | 110/112 (98%)  | 0.31   | 1 (0%) 84 85 | 34, 45, 56, 65        | 0     |
| 14  | 2S    | 110/112 (98%)  | 0.48   | 9 (8%) 11 9  | 59, 69, 76, 81        | 0     |
| 15  | 1T    | 131/146 (89%)  | 0.30   | 1 (0%) 86 87 | 28, 38, 62, 75        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.33   | 1 (0%) 86 87 | 41, 52, 70, 76        | 0     |
| 16  | 1U    | 116/118 (98%)  | 0.63   | 1 (0%) 84 85 | 18, 25, 39, 57        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.79   | 9 (7%) 13 11 | 33, 52, 67, 74        | 0     |
| 17  | 1V    | 101/101 (100%) | 0.36   | 0 100 100    | 15, 35, 54, 67        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.44   | 3 (2%) 50 51 | 31, 62, 72, 77        | 0     |
| 18  | 1W    | 112/113 (99%)  | 0.46   | 1 (0%) 84 85 | 19, 27, 46, 75        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.67   | 8 (7%) 16 14 | 29, 43, 59, 84        | 0     |
| 19  | 1X    | 95/96 (98%)    | 0.44   | 1 (1%) 80 82 | 23, 32, 58, 68        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.68   | 5 (5%) 26 25 | 43, 54, 69, 74        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.39   | 1 (0%) 84 85 | 29, 42, 62, 67        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 1.10   | 15 (14%) 2 1 | 49, 63, 73, 82        | 0     |
| 21  | 1Z    | 203/206 (98%)  | 0.13   | 2 (0%) 82 83 | 35, 51, 66, 76        | 0     |
| 21  | 2Z    | 201/206 (97%)  | 0.21   | 8 (3%) 38 37 | 57, 71, 79, 88        | 0     |
| 22  | 10    | 77/85 (90%)    | 0.56   | 1 (1%) 77 78 | 24, 31, 48, 54        | 0     |
| 22  | 20    | 77/85 (90%)    | 0.99   | 12 (15%) 2 1 | 43, 57, 67, 72        | 0     |
| 23  | 11    | 97/98 (98%)    | 0.83   | 5 (5%) 27 25 | 22, 39, 61, 69        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.92   | 8 (8%) 11 9  | 35, 49, 71, 73        | 0     |
| 24  | 12    | 70/72 (97%)    | 0.24   | 1 (1%) 75 77 | 29, 44, 57, 78        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.40   | 2 (2%) 51 52 | 53, 64, 71, 73        | 0     |
| 25  | 13    | 59/60 (98%)    | 0.44   | 0 100 100    | 20, 30, 55, 63        | 0     |
| 25  | 23    | 59/60 (98%)    | 1.13   | 14 (23%) 0 0 | 45, 55, 69, 77        | 0     |
| 26  | 14    | 69/71 (97%)    | 0.22   | 4 (5%) 23 22 | 50, 69, 86, 90        | 0     |
| 26  | 24    | 69/71 (97%)    | 0.48   | 6 (8%) 10 8  | 70, 83, 88, 91        | 0     |
| 27  | 15    | 59/60 (98%)    | 0.53   | 0 100 100    | 17, 27, 44, 54        | 0     |
| 27  | 25    | 59/60 (98%)    | 0.38   | 2 (3%) 45 45 | 29, 44, 59, 68        | 0     |
| 28  | 16    | 53/54 (98%)    | 0.15   | 0 100 100    | 28, 36, 48, 55        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.30   | 0 100 100     | 46, 54, 63, 68        | 0     |
| 29  | 17    | 48/49 (97%)     | 0.90   | 2 (4%) 36 35  | 17, 24, 49, 58        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.85   | 4 (8%) 11 9   | 28, 36, 58, 65        | 0     |
| 30  | 18    | 64/65 (98%)     | 0.64   | 1 (1%) 72 74  | 23, 28, 34, 47        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.88   | 4 (6%) 20 19  | 38, 49, 56, 63        | 0     |
| 31  | 19    | 37/37 (100%)    | 0.56   | 1 (2%) 54 55  | 22, 32, 49, 53        | 0     |
| 31  | 29    | 37/37 (100%)    | 1.34   | 8 (21%) 0 0   | 50, 60, 68, 69        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.11   | 20 (1%) 77 78 | 32, 62, 89, 104       | 0     |
| 32  | 2a    | 1492/1521 (98%) | 0.13   | 23 (1%) 73 76 | 42, 71, 91, 103       | 0     |
| 33  | 1b    | 231/256 (90%)   | 0.33   | 9 (3%) 39 38  | 61, 74, 83, 88        | 0     |
| 33  | 2b    | 231/256 (90%)   | 0.72   | 34 (14%) 2 1  | 66, 80, 86, 90        | 0     |
| 34  | 1c    | 206/239 (86%)   | 0.55   | 11 (5%) 26 25 | 53, 67, 77, 81        | 0     |
| 34  | 2c    | 206/239 (86%)   | 0.92   | 31 (15%) 2 1  | 70, 79, 84, 91        | 0     |
| 35  | 1d    | 208/209 (99%)   | 0.72   | 20 (9%) 8 6   | 51, 66, 75, 81        | 0     |
| 35  | 2d    | 208/209 (99%)   | 1.14   | 39 (18%) 1 0  | 55, 68, 77, 79        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.49   | 4 (2%) 54 55  | 46, 59, 69, 80        | 0     |
| 36  | 2e    | 148/162 (91%)   | 0.82   | 20 (13%) 3 2  | 57, 68, 76, 83        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.27   | 1 (1%) 82 83  | 43, 60, 70, 74        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.02   | 0 100 100     | 52, 62, 70, 76        | 0     |
| 38  | 1g    | 155/156 (99%)   | 0.31   | 6 (3%) 39 38  | 56, 65, 76, 85        | 0     |
| 38  | 2g    | 155/156 (99%)   | 0.35   | 10 (6%) 18 17 | 68, 74, 81, 87        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.63   | 8 (5%) 23 22  | 51, 62, 71, 74        | 0     |
| 39  | 2h    | 137/138 (99%)   | 0.61   | 7 (5%) 28 26  | 58, 69, 74, 82        | 0     |
| 40  | 1i    | 127/128 (99%)   | 0.71   | 17 (13%) 3 2  | 52, 73, 79, 82        | 0     |
| 40  | 2i    | 126/128 (98%)   | 1.74   | 49 (38%) 0 0  | 67, 80, 85, 87        | 0     |
| 41  | 1j    | 97/105 (92%)    | 0.50   | 13 (13%) 3 2  | 52, 72, 83, 86        | 0     |
| 41  | 2j    | 96/105 (91%)    | 2.13   | 47 (48%) 0 0  | 71, 80, 85, 87        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.22   | 0 100 100     | 39, 58, 69, 73        | 0     |
| 42  | 2k    | 114/129 (88%)   | 0.62   | 7 (6%) 21 20  | 50, 66, 75, 81        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.46   | 4 (3%) 46 46  | 42, 54, 65, 70        | 0     |
| 43  | 2l    | 121/132 (91%)   | 0.97   | 16 (13%) 3 2  | 54, 62, 69, 77        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | 1m    | 116/126 (92%)     | 0.32   | 4 (3%) 45 45   | 52, 68, 75, 79        | 0     |
| 44  | 2m    | 114/126 (90%)     | 0.82   | 12 (10%) 6 4   | 73, 80, 85, 87        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.23   | 10 (16%) 1 1   | 57, 64, 72, 79        | 0     |
| 45  | 2n    | 60/61 (98%)       | 2.71   | 36 (60%) 0 0   | 71, 79, 85, 88        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.42   | 0 100 100      | 43, 60, 71, 77        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.61   | 2 (2%) 60 62   | 54, 67, 75, 78        | 0     |
| 47  | 1p    | 82/88 (93%)       | 1.04   | 12 (14%) 2 1   | 55, 67, 77, 80        | 0     |
| 47  | 2p    | 82/88 (93%)       | 0.80   | 8 (9%) 7 5     | 55, 65, 75, 82        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.49   | 6 (6%) 21 20   | 48, 63, 72, 73        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.55   | 7 (7%) 16 14   | 53, 63, 73, 79        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.26   | 1 (1%) 73 76   | 51, 60, 73, 76        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.35   | 2 (2%) 51 52   | 59, 67, 74, 76        | 0     |
| 50  | 1s    | 83/93 (89%)       | 0.14   | 1 (1%) 79 80   | 59, 70, 76, 79        | 0     |
| 50  | 2s    | 83/93 (89%)       | 0.98   | 15 (18%) 1 1   | 70, 82, 86, 88        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.78   | 15 (15%) 2 1   | 53, 66, 76, 82        | 0     |
| 51  | 2t    | 98/106 (92%)      | 0.45   | 7 (7%) 16 14   | 53, 64, 75, 77        | 0     |
| 52  | 1u    | 23/27 (85%)       | 1.77   | 9 (39%) 0 0    | 61, 66, 69, 72        | 0     |
| 52  | 2u    | 23/27 (85%)       | 2.31   | 14 (60%) 0 0   | 73, 76, 80, 82        | 0     |
| 53  | 1y    | 97/113 (85%)      | 0.62   | 4 (4%) 37 36   | 45, 56, 67, 71        | 0     |
| 53  | 2y    | 96/113 (84%)      | 2.26   | 51 (53%) 0 0   | 60, 72, 79, 83        | 0     |
| All | All   | 20766/21468 (96%) | 0.45   | 976 (4%) 31 30 | 15, 57, 84, 105       | 0     |

The worst 5 of 976 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 1110 | C    | 7.7  |
| 45  | 2n    | 59   | ALA  | 7.6  |
| 1   | 1A    | 1122 | C    | 7.4  |
| 40  | 2i    | 127  | LYS  | 7.3  |
| 1   | 1A    | 1133 | G    | 7.1  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.89 | 0.15 | 76,82,88,101               | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.90 | 0.25 | 63,68,77,88                | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.92 | 0.13 | 71,78,90,90                | 0     |
| 1   | PSU  | 1A    | 1939 | 20/21 | 0.92 | 0.17 | 62,68,77,77                | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.92 | 0.15 | 76,86,91,102               | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.92 | 0.28 | 60,65,71,95                | 0     |
| 1   | 5MU  | 1A    | 1937 | 21/22 | 0.93 | 0.17 | 67,74,83,94                | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.93 | 0.13 | 56,70,76,78                | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.93 | 0.22 | 57,67,81,92                | 0     |
| 1   | 4OC  | 2A    | 1920 | 21/23 | 0.94 | 0.17 | 61,65,72,73                | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.94 | 0.16 | 71,76,80,84                | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.94 | 0.23 | 50,54,59,76                | 0     |
| 1   | PSU  | 1A    | 1933 | 20/21 | 0.95 | 0.15 | 55,62,65,66                | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.95 | 0.17 | 56,60,64,65                | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.95 | 0.17 | 56,66,69,71                | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.95 | 0.20 | 53,63,68,71                | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.95 | 0.21 | 51,60,63,66                | 0     |
| 32  | 7MG  | 2a    | 527  | 24/25 | 0.95 | 0.18 | 61,67,73,74                | 0     |
| 32  | 7MG  | 1a    | 527  | 24/25 | 0.96 | 0.22 | 42,51,54,59                | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.96 | 0.18 | 50,60,64,68                | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.96 | 0.25 | 51,61,66,67                | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.96 | 0.19 | 53,58,65,71                | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.97 | 0.17 | 36,48,53,54                | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.97 | 0.29 | 65,70,73,74                | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.25 | 29,35,39,44                | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.97 | 0.19 | 43,46,52,60                | 0     |
| 1   | 4OC  | 1A    | 1942 | 21/23 | 0.97 | 0.21 | 39,54,59,60                | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.97 | 0.20 | 52,58,63,66                | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.97 | 0.18 | 51,53,58,61                | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.19 | 29,36,41,43                | 0     |
| 1   | 2MU  | 2A    | 2552 | 21/23 | 0.98 | 0.22 | 30,36,39,41                | 0     |
| 1   | 5MC  | 1A    | 1984 | 21/22 | 0.98 | 0.21 | 25,33,37,45                | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.98 | 0.24 | 34,41,46,51                | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.98 | 0.23 | 37,43,46,49                | 0     |
| 1   | 2MA  | 1A    | 2515 | 23/24 | 0.98 | 0.25 | 16,20,24,31                | 0     |
| 1   | PSU  | 1A    | 2617 | 20/21 | 0.98 | 0.20 | 18,22,28,28                | 0     |
| 1   | 5MC  | 1A    | 1964 | 21/22 | 0.98 | 0.20 | 26,32,38,47                | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.98 | 0.21 | 40,45,49,51                | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.98 | 0.18 | 42,47,55,56                | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.98 | 0.20 | 35,44,46,49                | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.98 | 0.19 | 36,45,49,56                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.98 | 0.19 | 33,43,48,58                | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.98 | 0.23 | 32,36,38,39                | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.98 | 0.26 | 51,60,64,67                | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.98 | 0.25 | 24,30,35,37                | 0     |
| 1   | 2MU  | 1A    | 2564 | 21/23 | 0.99 | 0.21 | 20,26,28,29                | 0     |
| 1   | OMG  | 1A    | 2263 | 24/25 | 0.99 | 0.23 | 15,21,23,26                | 0     |
| 1   | 5MU  | 1A    | 1961 | 21/22 | 0.99 | 0.20 | 18,24,27,32                | 0     |

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 2A    | 3219 | 1/1   | 0.40 | 0.21 | 74,74,74,74                | 0     |
| 54  | MG   | 1a    | 1851 | 1/1   | 0.42 | 0.65 | 94,94,94,94                | 0     |
| 54  | MG   | 2A    | 3167 | 1/1   | 0.43 | 0.24 | 74,74,74,74                | 0     |
| 54  | MG   | 2B    | 3007 | 1/1   | 0.47 | 0.27 | 71,71,71,71                | 0     |
| 54  | MG   | 1a    | 1840 | 1/1   | 0.48 | 0.20 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3197 | 1/1   | 0.49 | 0.23 | 73,73,73,73                | 0     |
| 54  | MG   | 2A    | 3215 | 1/1   | 0.51 | 0.18 | 73,73,73,73                | 0     |
| 54  | MG   | 1a    | 1828 | 1/1   | 0.54 | 0.18 | 62,62,62,62                | 0     |
| 54  | MG   | 2B    | 3015 | 1/1   | 0.56 | 0.19 | 74,74,74,74                | 0     |
| 54  | MG   | 2A    | 3692 | 1/1   | 0.61 | 0.19 | 63,63,63,63                | 0     |
| 54  | MG   | 2A    | 3703 | 1/1   | 0.61 | 0.12 | 81,81,81,81                | 0     |
| 54  | MG   | 1A    | 3191 | 1/1   | 0.62 | 0.26 | 51,51,51,51                | 0     |
| 54  | MG   | 2a    | 1684 | 1/1   | 0.62 | 0.13 | 60,60,60,60                | 0     |
| 54  | MG   | 1B    | 219  | 1/1   | 0.63 | 0.13 | 46,46,46,46                | 0     |
| 54  | MG   | 1B    | 211  | 1/1   | 0.63 | 0.18 | 64,64,64,64                | 0     |
| 54  | MG   | 2a    | 1662 | 1/1   | 0.63 | 0.22 | 67,67,67,67                | 0     |
| 54  | MG   | 2A    | 3142 | 1/1   | 0.63 | 0.18 | 68,68,68,68                | 0     |
| 54  | MG   | 2A    | 3318 | 1/1   | 0.64 | 0.19 | 78,78,78,78                | 0     |
| 54  | MG   | 2A    | 3338 | 1/1   | 0.65 | 0.19 | 53,53,53,53                | 0     |
| 54  | MG   | 1a    | 1830 | 1/1   | 0.66 | 0.21 | 66,66,66,66                | 0     |
| 54  | MG   | 20    | 101  | 1/1   | 0.66 | 0.21 | 75,75,75,75                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3160 | 1/1   | 0.67 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3934 | 1/1   | 0.67 | 0.39 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3189 | 1/1   | 0.67 | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1766 | 1/1   | 0.68 | 0.28 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3278 | 1/1   | 0.68 | 0.22 | 38,38,38,38                 | 0     |
| 54  | MG   | 1a    | 1684 | 1/1   | 0.68 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1640 | 1/1   | 0.69 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3327 | 1/1   | 0.69 | 0.19 | 33,33,33,33                 | 0     |
| 54  | MG   | 2a    | 1611 | 1/1   | 0.69 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 1645 | 1/1   | 0.69 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3982 | 1/1   | 0.69 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1793 | 1/1   | 0.69 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3346 | 1/1   | 0.70 | 0.18 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1624 | 1/1   | 0.70 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3567 | 1/1   | 0.70 | 0.18 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3206 | 1/1   | 0.70 | 0.45 | 45,45,45,45                 | 0     |
| 54  | MG   | 1d    | 307  | 1/1   | 0.70 | 0.14 | 89,89,89,89                 | 0     |
| 54  | MG   | 2A    | 3173 | 1/1   | 0.70 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3921 | 1/1   | 0.71 | 0.41 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1608 | 1/1   | 0.71 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3986 | 1/1   | 0.71 | 0.34 | 61,61,61,61                 | 0     |
| 54  | MG   | 1B    | 207  | 1/1   | 0.71 | 0.21 | 41,41,41,41                 | 0     |
| 54  | MG   | 2I    | 3001 | 1/1   | 0.71 | 0.17 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3171 | 1/1   | 0.71 | 0.28 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1677 | 1/1   | 0.71 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3393 | 1/1   | 0.71 | 0.15 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3804 | 1/1   | 0.71 | 0.12 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3635 | 1/1   | 0.71 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3756 | 1/1   | 0.72 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3259 | 1/1   | 0.72 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3398 | 1/1   | 0.72 | 0.15 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3422 | 1/1   | 0.72 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1797 | 1/1   | 0.72 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | 2I    | 101  | 1/1   | 0.73 | 0.13 | 67,67,67,67                 | 0     |
| 54  | MG   | 1y    | 3002 | 1/1   | 0.73 | 0.25 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3575 | 1/1   | 0.73 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3597 | 1/1   | 0.73 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 1673 | 1/1   | 0.73 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3184 | 1/1   | 0.73 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3805 | 1/1   | 0.74 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1681 | 1/1   | 0.74 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1652 | 1/1   | 0.74 | 0.14 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3103 | 1/1   | 0.74 | 0.27 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3198 | 1/1   | 0.74 | 0.22 | 60,60,60,60                 | 0     |
| 54  | MG   | 2Q    | 3002 | 1/1   | 0.75 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3297 | 1/1   | 0.75 | 0.21 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3676 | 1/1   | 0.75 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 1F    | 311  | 1/1   | 0.75 | 0.51 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3941 | 1/1   | 0.75 | 0.23 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3950 | 1/1   | 0.75 | 0.14 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3488 | 1/1   | 0.75 | 0.08 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3957 | 1/1   | 0.75 | 0.32 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3279 | 1/1   | 0.76 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3894 | 1/1   | 0.76 | 0.38 | 80,80,80,80                 | 0     |
| 54  | MG   | 1a    | 1700 | 1/1   | 0.76 | 0.21 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1834 | 1/1   | 0.76 | 0.29 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1752 | 1/1   | 0.76 | 0.17 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3662 | 1/1   | 0.76 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 1638 | 1/1   | 0.76 | 0.19 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 1642 | 1/1   | 0.76 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3685 | 1/1   | 0.76 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1680 | 1/1   | 0.76 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3274 | 1/1   | 0.76 | 0.26 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3175 | 1/1   | 0.76 | 0.20 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 1742 | 1/1   | 0.76 | 0.25 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1606 | 1/1   | 0.77 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1637 | 1/1   | 0.77 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3702 | 1/1   | 0.77 | 0.16 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3098 | 1/1   | 0.77 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1835 | 1/1   | 0.77 | 0.25 | 67,67,67,67                 | 0     |
| 54  | MG   | 2B    | 3001 | 1/1   | 0.77 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1737 | 1/1   | 0.77 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3195 | 1/1   | 0.77 | 0.21 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1843 | 1/1   | 0.77 | 0.09 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3166 | 1/1   | 0.77 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1748 | 1/1   | 0.78 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3405 | 1/1   | 0.78 | 0.17 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3783 | 1/1   | 0.78 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 2W    | 8002 | 1/1   | 0.78 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3177 | 1/1   | 0.78 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3216 | 1/1   | 0.78 | 0.21 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 1604 | 1/1   | 0.78 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3673 | 1/1   | 0.78 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 1630 | 1/1   | 0.78 | 0.12 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1A    | 3794 | 1/1   | 0.78 | 0.14 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3744 | 1/1   | 0.78 | 0.13 | 54,54,54,54                | 0     |
| 54  | MG   | 2A    | 3095 | 1/1   | 0.78 | 0.13 | 58,58,58,58                | 0     |
| 54  | MG   | 2A    | 3332 | 1/1   | 0.78 | 0.14 | 65,65,65,65                | 0     |
| 54  | MG   | 1A    | 3576 | 1/1   | 0.78 | 0.12 | 43,43,43,43                | 0     |
| 54  | MG   | 2A    | 3389 | 1/1   | 0.78 | 0.23 | 47,47,47,47                | 0     |
| 54  | MG   | 2B    | 3014 | 1/1   | 0.78 | 0.17 | 71,71,71,71                | 0     |
| 54  | MG   | 1a    | 1782 | 1/1   | 0.79 | 0.22 | 61,61,61,61                | 0     |
| 54  | MG   | 1A    | 3473 | 1/1   | 0.79 | 0.10 | 63,63,63,63                | 0     |
| 54  | MG   | 2A    | 3146 | 1/1   | 0.79 | 0.48 | 52,52,52,52                | 0     |
| 54  | MG   | 2A    | 3226 | 1/1   | 0.79 | 0.23 | 53,53,53,53                | 0     |
| 54  | MG   | 2A    | 3149 | 1/1   | 0.79 | 0.12 | 68,68,68,68                | 0     |
| 54  | MG   | 1a    | 1668 | 1/1   | 0.79 | 0.25 | 74,74,74,74                | 0     |
| 54  | MG   | 1a    | 1802 | 1/1   | 0.79 | 0.18 | 62,62,62,62                | 0     |
| 54  | MG   | 1a    | 1674 | 1/1   | 0.79 | 0.13 | 65,65,65,65                | 0     |
| 54  | MG   | 2A    | 3385 | 1/1   | 0.79 | 0.13 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3011 | 1/1   | 0.79 | 0.18 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3383 | 1/1   | 0.79 | 0.13 | 24,24,24,24                | 0     |
| 54  | MG   | 1D    | 309  | 1/1   | 0.79 | 0.13 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3938 | 1/1   | 0.79 | 0.17 | 64,64,64,64                | 0     |
| 54  | MG   | 1A    | 3100 | 1/1   | 0.79 | 0.26 | 39,39,39,39                | 0     |
| 54  | MG   | 1A    | 3603 | 1/1   | 0.79 | 0.15 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3649 | 1/1   | 0.79 | 0.14 | 58,58,58,58                | 0     |
| 54  | MG   | 1A    | 3189 | 1/1   | 0.79 | 0.42 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 3835 | 1/1   | 0.79 | 0.12 | 50,50,50,50                | 0     |
| 54  | MG   | 1a    | 1767 | 1/1   | 0.79 | 0.42 | 58,58,58,58                | 0     |
| 54  | MG   | 2a    | 1689 | 1/1   | 0.79 | 0.24 | 62,62,62,62                | 0     |
| 54  | MG   | 2a    | 1737 | 1/1   | 0.79 | 0.18 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3694 | 1/1   | 0.79 | 0.27 | 69,69,69,69                | 0     |
| 58  | ARG  | 1F    | 314  | 12/12 | 0.79 | 0.23 | 47,65,78,79                | 0     |
| 54  | MG   | 2A    | 3553 | 1/1   | 0.80 | 0.16 | 56,56,56,56                | 0     |
| 54  | MG   | 1d    | 301  | 1/1   | 0.80 | 0.11 | 68,68,68,68                | 0     |
| 54  | MG   | 2A    | 3589 | 1/1   | 0.80 | 0.16 | 57,57,57,57                | 0     |
| 54  | MG   | 2A    | 3608 | 1/1   | 0.80 | 0.11 | 40,40,40,40                | 0     |
| 54  | MG   | 2A    | 3621 | 1/1   | 0.80 | 0.14 | 28,28,28,28                | 0     |
| 54  | MG   | 2A    | 3304 | 1/1   | 0.80 | 0.10 | 44,44,44,44                | 0     |
| 54  | MG   | 1A    | 3870 | 1/1   | 0.80 | 0.11 | 46,46,46,46                | 0     |
| 54  | MG   | 2a    | 1613 | 1/1   | 0.80 | 0.17 | 51,51,51,51                | 0     |
| 54  | MG   | 1y    | 3001 | 1/1   | 0.80 | 0.38 | 61,61,61,61                | 0     |
| 54  | MG   | 1a    | 1653 | 1/1   | 0.80 | 0.16 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3594 | 1/1   | 0.80 | 0.17 | 54,54,54,54                | 0     |
| 54  | MG   | 2A    | 3386 | 1/1   | 0.80 | 0.14 | 68,68,68,68                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3697 | 1/1   | 0.80 | 0.11 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3159 | 1/1   | 0.80 | 0.19 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3782 | 1/1   | 0.80 | 0.11 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3398 | 1/1   | 0.80 | 0.28 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3577 | 1/1   | 0.80 | 0.20 | 26,26,26,26                 | 0     |
| 54  | MG   | 1a    | 1824 | 1/1   | 0.80 | 0.20 | 55,55,55,55                 | 0     |
| 54  | MG   | 2B    | 3018 | 1/1   | 0.80 | 0.27 | 76,76,76,76                 | 0     |
| 54  | MG   | 2X    | 101  | 1/1   | 0.81 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3330 | 1/1   | 0.81 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1754 | 1/1   | 0.81 | 0.23 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3193 | 1/1   | 0.81 | 0.27 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 1605 | 1/1   | 0.81 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3355 | 1/1   | 0.81 | 0.23 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3187 | 1/1   | 0.81 | 0.39 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3047 | 1/1   | 0.81 | 0.51 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3858 | 1/1   | 0.81 | 0.14 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1629 | 1/1   | 0.81 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3602 | 1/1   | 0.81 | 0.20 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3779 | 1/1   | 0.81 | 0.24 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1720 | 1/1   | 0.81 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 1682 | 1/1   | 0.81 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3913 | 1/1   | 0.81 | 0.32 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3962 | 1/1   | 0.81 | 0.08 | 55,55,55,55                 | 0     |
| 54  | MG   | 1R    | 203  | 1/1   | 0.81 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3188 | 1/1   | 0.81 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1748 | 1/1   | 0.81 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 2q    | 201  | 1/1   | 0.81 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3326 | 1/1   | 0.81 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3242 | 1/1   | 0.82 | 0.41 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3271 | 1/1   | 0.82 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3445 | 1/1   | 0.82 | 0.10 | 21,21,21,21                 | 0     |
| 54  | MG   | 2a    | 1602 | 1/1   | 0.82 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3330 | 1/1   | 0.82 | 0.17 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3908 | 1/1   | 0.82 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3640 | 1/1   | 0.82 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1701 | 1/1   | 0.82 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | 2a    | 1615 | 1/1   | 0.82 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 1623 | 1/1   | 0.82 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3637 | 1/1   | 0.82 | 0.38 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3789 | 1/1   | 0.82 | 0.22 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3151 | 1/1   | 0.82 | 0.47 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3380 | 1/1   | 0.82 | 0.15 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 1648 | 1/1   | 0.82 | 0.11 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3203 | 1/1   | 0.82 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3165 | 1/1   | 0.82 | 0.28 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 1676 | 1/1   | 0.82 | 0.21 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1667 | 1/1   | 0.82 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3138 | 1/1   | 0.82 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3144 | 1/1   | 0.82 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1709 | 1/1   | 0.82 | 0.32 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3449 | 1/1   | 0.82 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 10    | 105  | 1/1   | 0.82 | 0.21 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 1747 | 1/1   | 0.82 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3544 | 1/1   | 0.82 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3229 | 1/1   | 0.82 | 0.66 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3563 | 1/1   | 0.82 | 0.11 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3112 | 1/1   | 0.83 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3116 | 1/1   | 0.83 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3635 | 1/1   | 0.83 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1783 | 1/1   | 0.83 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | 1N    | 202  | 1/1   | 0.83 | 0.18 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3836 | 1/1   | 0.83 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1679 | 1/1   | 0.83 | 0.22 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3341 | 1/1   | 0.83 | 0.15 | 33,33,33,33                 | 0     |
| 54  | MG   | 1a    | 1813 | 1/1   | 0.83 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3039 | 1/1   | 0.83 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1604 | 1/1   | 0.83 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3479 | 1/1   | 0.83 | 0.18 | 20,20,20,20                 | 0     |
| 54  | MG   | 1a    | 1686 | 1/1   | 0.83 | 0.23 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3961 | 1/1   | 0.83 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3567 | 1/1   | 0.83 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1707 | 1/1   | 0.83 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3472 | 1/1   | 0.83 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3899 | 1/1   | 0.83 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3502 | 1/1   | 0.83 | 0.27 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3520 | 1/1   | 0.83 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3194 | 1/1   | 0.83 | 0.21 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3548 | 1/1   | 0.83 | 0.15 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3194 | 1/1   | 0.83 | 0.16 | 60,60,60,60                 | 0     |
| 54  | MG   | 1d    | 303  | 1/1   | 0.83 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3735 | 1/1   | 0.83 | 0.12 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3569 | 1/1   | 0.83 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1669 | 1/1   | 0.83 | 0.19 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1749 | 1/1   | 0.83 | 0.13 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3737 | 1/1   | 0.83 | 0.24 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 1678 | 1/1   | 0.83 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3619 | 1/1   | 0.83 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | 1y    | 3004 | 1/1   | 0.83 | 0.28 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3053 | 1/1   | 0.83 | 0.28 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3056 | 1/1   | 0.83 | 0.32 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3060 | 1/1   | 0.83 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3927 | 1/1   | 0.83 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1662 | 1/1   | 0.83 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3691 | 1/1   | 0.83 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 2p    | 3001 | 1/1   | 0.83 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3190 | 1/1   | 0.83 | 0.19 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3251 | 1/1   | 0.83 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3401 | 1/1   | 0.84 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1676 | 1/1   | 0.84 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3428 | 1/1   | 0.84 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3825 | 1/1   | 0.84 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3499 | 1/1   | 0.84 | 0.40 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3202 | 1/1   | 0.84 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3072 | 1/1   | 0.84 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3508 | 1/1   | 0.84 | 0.22 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3748 | 1/1   | 0.84 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3214 | 1/1   | 0.84 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3854 | 1/1   | 0.84 | 0.15 | 19,19,19,19                 | 0     |
| 54  | MG   | 1a    | 1612 | 1/1   | 0.84 | 0.11 | 72,72,72,72                 | 0     |
| 54  | MG   | 2a    | 1614 | 1/1   | 0.84 | 0.21 | 74,74,74,74                 | 0     |
| 54  | MG   | 1a    | 1814 | 1/1   | 0.84 | 0.23 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1617 | 1/1   | 0.84 | 0.15 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1620 | 1/1   | 0.84 | 0.14 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3587 | 1/1   | 0.84 | 0.48 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 4023 | 1/1   | 0.84 | 0.49 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1833 | 1/1   | 0.84 | 0.29 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1704 | 1/1   | 0.84 | 0.18 | 77,77,77,77                 | 0     |
| 54  | MG   | 2a    | 1656 | 1/1   | 0.84 | 0.08 | 63,63,63,63                 | 0     |
| 54  | MG   | 1B    | 202  | 1/1   | 0.84 | 0.23 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3308 | 1/1   | 0.84 | 0.15 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1715 | 1/1   | 0.84 | 0.20 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3658 | 1/1   | 0.84 | 0.15 | 34,34,34,34                 | 0     |
| 54  | MG   | 1B    | 206  | 1/1   | 0.84 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1846 | 1/1   | 0.84 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3214 | 1/1   | 0.84 | 0.30 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3335 | 1/1   | 0.84 | 0.19 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 1700 | 1/1   | 0.84 | 0.21 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3373 | 1/1   | 0.84 | 0.15 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3177 | 1/1   | 0.84 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3949 | 1/1   | 0.84 | 0.28 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3817 | 1/1   | 0.84 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3951 | 1/1   | 0.84 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 2j    | 8001 | 1/1   | 0.84 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | 2A    | 3191 | 1/1   | 0.84 | 0.23 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3903 | 1/1   | 0.84 | 0.22 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3014 | 1/1   | 0.84 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 2B    | 3013 | 1/1   | 0.85 | 0.16 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3096 | 1/1   | 0.85 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1U    | 202  | 1/1   | 0.85 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3447 | 1/1   | 0.85 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 2D    | 305  | 1/1   | 0.85 | 0.20 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3798 | 1/1   | 0.85 | 0.18 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3467 | 1/1   | 0.85 | 0.15 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3430 | 1/1   | 0.85 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3476 | 1/1   | 0.85 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3486 | 1/1   | 0.85 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3434 | 1/1   | 0.85 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3218 | 1/1   | 0.85 | 0.23 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3173 | 1/1   | 0.85 | 0.17 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3379 | 1/1   | 0.85 | 0.13 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1755 | 1/1   | 0.85 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3303 | 1/1   | 0.85 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3552 | 1/1   | 0.85 | 0.10 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3208 | 1/1   | 0.85 | 0.13 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3273 | 1/1   | 0.85 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1777 | 1/1   | 0.85 | 0.21 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 1631 | 1/1   | 0.85 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3303 | 1/1   | 0.85 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3581 | 1/1   | 0.85 | 0.19 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3527 | 1/1   | 0.85 | 0.09 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3170 | 1/1   | 0.85 | 0.28 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3314 | 1/1   | 0.85 | 0.13 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3610 | 1/1   | 0.85 | 0.22 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3618 | 1/1   | 0.85 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 1t    | 3001 | 1/1   | 0.85 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1628 | 1/1   | 0.85 | 0.18 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3563 | 1/1   | 0.85 | 0.25 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3209 | 1/1   | 0.85 | 0.18 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3887 | 1/1   | 0.85 | 0.06 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3667 | 1/1   | 0.85 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3021 | 1/1   | 0.85 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3036 | 1/1   | 0.85 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 1726 | 1/1   | 0.85 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 1729 | 1/1   | 0.85 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3350 | 1/1   | 0.85 | 0.16 | 31,31,31,31                 | 0     |
| 54  | MG   | 1a    | 1810 | 1/1   | 0.85 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1702 | 1/1   | 0.85 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3056 | 1/1   | 0.85 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3663 | 1/1   | 0.85 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3080 | 1/1   | 0.85 | 0.23 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3087 | 1/1   | 0.85 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1659 | 1/1   | 0.85 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 1D    | 310  | 1/1   | 0.86 | 0.22 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1775 | 1/1   | 0.86 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1776 | 1/1   | 0.86 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3430 | 1/1   | 0.86 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3131 | 1/1   | 0.86 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1780 | 1/1   | 0.86 | 0.25 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1671 | 1/1   | 0.86 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 1G    | 3003 | 1/1   | 0.86 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3339 | 1/1   | 0.86 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1794 | 1/1   | 0.86 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3867 | 1/1   | 0.86 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3493 | 1/1   | 0.86 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3720 | 1/1   | 0.86 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3953 | 1/1   | 0.86 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 17    | 102  | 1/1   | 0.86 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3521 | 1/1   | 0.86 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1607 | 1/1   | 0.86 | 0.19 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3875 | 1/1   | 0.86 | 0.31 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1817 | 1/1   | 0.86 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3730 | 1/1   | 0.86 | 0.16 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3488 | 1/1   | 0.86 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 1618 | 1/1   | 0.86 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3262 | 1/1   | 0.86 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 1627 | 1/1   | 0.86 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3126 | 1/1   | 0.86 | 0.22 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3137 | 1/1   | 0.86 | 0.21 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3579 | 1/1   | 0.86 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3969 | 1/1   | 0.86 | 0.34 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3799 | 1/1   | 0.86 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3147 | 1/1   | 0.86 | 0.68 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3590 | 1/1   | 0.86 | 0.58 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3901 | 1/1   | 0.86 | 0.14 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 1663 | 1/1   | 0.86 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3233 | 1/1   | 0.86 | 0.38 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3321 | 1/1   | 0.86 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3082 | 1/1   | 0.86 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1841 | 1/1   | 0.86 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 1B    | 204  | 1/1   | 0.86 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3642 | 1/1   | 0.86 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1685 | 1/1   | 0.86 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3752 | 1/1   | 0.86 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1855 | 1/1   | 0.86 | 0.07 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 1704 | 1/1   | 0.86 | 0.28 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3669 | 1/1   | 0.86 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3672 | 1/1   | 0.86 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1641 | 1/1   | 0.86 | 0.22 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3675 | 1/1   | 0.86 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3584 | 1/1   | 0.86 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3183 | 1/1   | 0.86 | 0.32 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3559 | 1/1   | 0.86 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 1l    | 3002 | 1/1   | 0.86 | 0.21 | 72,72,72,72                 | 0     |
| 54  | MG   | 1B    | 224  | 1/1   | 0.86 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3847 | 1/1   | 0.86 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MPD  | 2A    | 3710 | 8/8   | 0.86 | 0.40 | 43,49,51,57                 | 0     |
| 57  | MPD  | 2B    | 3020 | 8/8   | 0.86 | 0.26 | 61,66,69,79                 | 0     |
| 54  | MG   | 2A    | 3399 | 1/1   | 0.86 | 0.15 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3684 | 1/1   | 0.87 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3370 | 1/1   | 0.87 | 0.10 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3172 | 1/1   | 0.87 | 0.22 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3757 | 1/1   | 0.87 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3519 | 1/1   | 0.87 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 4017 | 1/1   | 0.87 | 0.20 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3397 | 1/1   | 0.87 | 0.35 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3280 | 1/1   | 0.87 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 1f    | 3002 | 1/1   | 0.87 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1633 | 1/1   | 0.87 | 0.16 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3291 | 1/1   | 0.87 | 0.17 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3421 | 1/1   | 0.87 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3158 | 1/1   | 0.87 | 0.23 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3031 | 1/1   | 0.87 | 0.25 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1773 | 1/1   | 0.87 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | 2P    | 202  | 1/1   | 0.87 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3448 | 1/1   | 0.87 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3010 | 1/1   | 0.87 | 0.26 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3466 | 1/1   | 0.87 | 0.14 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1649 | 1/1   | 0.87 | 0.43 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1650 | 1/1   | 0.87 | 0.22 | 62,62,62,62                 | 0     |
| 54  | MG   | 28    | 8002 | 1/1   | 0.87 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 28    | 8003 | 1/1   | 0.87 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3906 | 1/1   | 0.87 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 1603 | 1/1   | 0.87 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3477 | 1/1   | 0.87 | 0.34 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3665 | 1/1   | 0.87 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1658 | 1/1   | 0.87 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3670 | 1/1   | 0.87 | 0.18 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3068 | 1/1   | 0.87 | 0.44 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3071 | 1/1   | 0.87 | 0.31 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3510 | 1/1   | 0.87 | 0.21 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3675 | 1/1   | 0.87 | 0.16 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3078 | 1/1   | 0.87 | 0.08 | 63,63,63,63                 | 0     |
| 54  | MG   | 1D    | 302  | 1/1   | 0.87 | 0.42 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3545 | 1/1   | 0.87 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3547 | 1/1   | 0.87 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3252 | 1/1   | 0.87 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1639 | 1/1   | 0.87 | 0.28 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3231 | 1/1   | 0.87 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3095 | 1/1   | 0.87 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1805 | 1/1   | 0.87 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1651 | 1/1   | 0.87 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3252 | 1/1   | 0.87 | 0.23 | 61,61,61,61                 | 0     |
| 54  | MG   | 1E    | 305  | 1/1   | 0.87 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3937 | 1/1   | 0.87 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | 1G    | 3002 | 1/1   | 0.87 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3285 | 1/1   | 0.87 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 1675 | 1/1   | 0.87 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3043 | 1/1   | 0.87 | 0.25 | 52,52,52,52                 | 0     |
| 54  | MG   | 1H    | 8001 | 1/1   | 0.87 | 0.16 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 1681 | 1/1   | 0.87 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3599 | 1/1   | 0.87 | 0.15 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 1683 | 1/1   | 0.87 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3305 | 1/1   | 0.87 | 0.16 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3832 | 1/1   | 0.87 | 0.13 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3943 | 1/1   | 0.87 | 0.20 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1694 | 1/1   | 0.87 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1832 | 1/1   | 0.87 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3440 | 1/1   | 0.87 | 0.17 | 18,18,18,18                 | 0     |
| 54  | MG   | 2A    | 3629 | 1/1   | 0.87 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1716 | 1/1   | 0.87 | 0.25 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3148 | 1/1   | 0.87 | 0.74 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3342 | 1/1   | 0.87 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3651 | 1/1   | 0.87 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3182 | 1/1   | 0.87 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3659 | 1/1   | 0.87 | 0.41 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3354 | 1/1   | 0.87 | 0.14 | 20,20,20,20                 | 0     |
| 54  | MG   | 2a    | 1749 | 1/1   | 0.87 | 0.27 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3361 | 1/1   | 0.87 | 0.19 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3866 | 1/1   | 0.87 | 0.10 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3755 | 1/1   | 0.87 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3120 | 1/1   | 0.87 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3368 | 1/1   | 0.87 | 0.15 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3683 | 1/1   | 0.87 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3562 | 1/1   | 0.88 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3917 | 1/1   | 0.88 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1791 | 1/1   | 0.88 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3619 | 1/1   | 0.88 | 0.42 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3402 | 1/1   | 0.88 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3550 | 1/1   | 0.88 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3029 | 1/1   | 0.88 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3935 | 1/1   | 0.88 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3041 | 1/1   | 0.88 | 0.16 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3093 | 1/1   | 0.88 | 0.20 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3602 | 1/1   | 0.88 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3192 | 1/1   | 0.88 | 0.19 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1808 | 1/1   | 0.88 | 0.19 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3274 | 1/1   | 0.88 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3355 | 1/1   | 0.88 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | 1a    | 1627 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1816 | 1/1   | 0.88 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1632 | 1/1   | 0.88 | 0.20 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3632 | 1/1   | 0.88 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3572 | 1/1   | 0.88 | 0.56 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 1641 | 1/1   | 0.88 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3324 | 1/1   | 0.88 | 0.20 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 1644 | 1/1   | 0.88 | 0.25 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3648 | 1/1   | 0.88 | 0.08 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3408 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3412 | 1/1   | 0.88 | 0.18 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3081 | 1/1   | 0.88 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3662 | 1/1   | 0.88 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3423 | 1/1   | 0.88 | 0.13 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 1667 | 1/1   | 0.88 | 0.27 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1631 | 1/1   | 0.88 | 0.26 | 64,64,64,64                 | 0     |
| 54  | MG   | 1D    | 307  | 1/1   | 0.88 | 0.18 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1635 | 1/1   | 0.88 | 0.19 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1729 | 1/1   | 0.88 | 0.25 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1731 | 1/1   | 0.88 | 0.24 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3106 | 1/1   | 0.88 | 0.22 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3111 | 1/1   | 0.88 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3242 | 1/1   | 0.88 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3672 | 1/1   | 0.88 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3124 | 1/1   | 0.88 | 0.27 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3481 | 1/1   | 0.88 | 0.46 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3695 | 1/1   | 0.88 | 0.15 | 36,36,36,36                 | 0     |
| 54  | MG   | 2a    | 1695 | 1/1   | 0.88 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3448 | 1/1   | 0.88 | 0.15 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3134 | 1/1   | 0.88 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3721 | 1/1   | 0.88 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1842 | 1/1   | 0.88 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 1F    | 310  | 1/1   | 0.88 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3055 | 1/1   | 0.88 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3332 | 1/1   | 0.88 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3258 | 1/1   | 0.88 | 0.24 | 32,32,32,32                 | 0     |
| 54  | MG   | 2a    | 1745 | 1/1   | 0.88 | 0.19 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3964 | 1/1   | 0.88 | 0.75 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3540 | 1/1   | 0.88 | 0.23 | 37,37,37,37                 | 0     |
| 54  | MG   | 2G    | 3003 | 1/1   | 0.88 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | 2f    | 3001 | 1/1   | 0.88 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3394 | 1/1   | 0.88 | 0.15 | 18,18,18,18                 | 0     |
| 54  | MG   | 1P    | 202  | 1/1   | 0.88 | 0.12 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3181 | 1/1   | 0.88 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3618 | 1/1   | 0.88 | 0.13 | 42,42,42,42                 | 0     |
| 54  | MG   | 1X    | 101  | 1/1   | 0.88 | 0.19 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 4010 | 1/1   | 0.88 | 0.74 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3055 | 1/1   | 0.89 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3205 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3468 | 1/1   | 0.89 | 0.16 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2D    | 301  | 1/1   | 0.89 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3690 | 1/1   | 0.89 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 2D    | 307  | 1/1   | 0.89 | 0.50 | 43,43,43,43                 | 0     |
| 54  | MG   | 1G    | 3001 | 1/1   | 0.89 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3820 | 1/1   | 0.89 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3205 | 1/1   | 0.89 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3703 | 1/1   | 0.89 | 0.36 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3705 | 1/1   | 0.89 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3708 | 1/1   | 0.89 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3718 | 1/1   | 0.89 | 0.13 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3230 | 1/1   | 0.89 | 0.30 | 55,55,55,55                 | 0     |
| 54  | MG   | 1S    | 8001 | 1/1   | 0.89 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1U    | 201  | 1/1   | 0.89 | 0.37 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 1601 | 1/1   | 0.89 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3245 | 1/1   | 0.89 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3524 | 1/1   | 0.89 | 0.21 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3538 | 1/1   | 0.89 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3958 | 1/1   | 0.89 | 0.20 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3484 | 1/1   | 0.89 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3258 | 1/1   | 0.89 | 0.11 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3124 | 1/1   | 0.89 | 0.20 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3184 | 1/1   | 0.89 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 19    | 502  | 1/1   | 0.89 | 0.21 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3280 | 1/1   | 0.89 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3500 | 1/1   | 0.89 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3287 | 1/1   | 0.89 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3296 | 1/1   | 0.89 | 0.10 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3301 | 1/1   | 0.89 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3611 | 1/1   | 0.89 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3399 | 1/1   | 0.89 | 0.16 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 4007 | 1/1   | 0.89 | 0.33 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3749 | 1/1   | 0.89 | 0.19 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1619 | 1/1   | 0.89 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3593 | 1/1   | 0.89 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3594 | 1/1   | 0.89 | 0.25 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3526 | 1/1   | 0.89 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 1649 | 1/1   | 0.89 | 0.16 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1844 | 1/1   | 0.89 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1622 | 1/1   | 0.89 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1742 | 1/1   | 0.89 | 0.25 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1743 | 1/1   | 0.89 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3156 | 1/1   | 0.89 | 0.12 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3030 | 1/1   | 0.89 | 0.09 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3530 | 1/1   | 0.89 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3348 | 1/1   | 0.89 | 0.19 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3633 | 1/1   | 0.89 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3404 | 1/1   | 0.89 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 1680 | 1/1   | 0.89 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3220 | 1/1   | 0.89 | 0.40 | 31,31,31,31                 | 0     |
| 54  | MG   | 1h    | 3002 | 1/1   | 0.89 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3654 | 1/1   | 0.89 | 0.48 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3375 | 1/1   | 0.89 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3384 | 1/1   | 0.89 | 0.39 | 38,38,38,38                 | 0     |
| 54  | MG   | 1n    | 502  | 1/1   | 0.89 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1693 | 1/1   | 0.89 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 1o    | 3001 | 1/1   | 0.89 | 0.18 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3161 | 1/1   | 0.89 | 0.16 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3241 | 1/1   | 0.89 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3010 | 1/1   | 0.89 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1B    | 229  | 1/1   | 0.89 | 0.11 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3122 | 1/1   | 0.89 | 0.13 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3253 | 1/1   | 0.89 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3016 | 1/1   | 0.89 | 0.62 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3019 | 1/1   | 0.89 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3687 | 1/1   | 0.89 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3123 | 1/1   | 0.89 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 2a    | 1746 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1781 | 1/1   | 0.89 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3936 | 1/1   | 0.89 | 0.36 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3196 | 1/1   | 0.89 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | 2e    | 3001 | 1/1   | 0.89 | 0.32 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3679 | 1/1   | 0.89 | 0.29 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3044 | 1/1   | 0.89 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3200 | 1/1   | 0.89 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3810 | 1/1   | 0.89 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3450 | 1/1   | 0.89 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 2B    | 3010 | 1/1   | 0.89 | 0.14 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3463 | 1/1   | 0.89 | 0.14 | 62,62,62,62                 | 0     |
| 59  | ZN   | 2Y    | 501  | 1/1   | 0.89 | 0.12 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3528 | 1/1   | 0.90 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3781 | 1/1   | 0.90 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3071 | 1/1   | 0.90 | 0.49 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3534 | 1/1   | 0.90 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3784 | 1/1   | 0.90 | 0.11 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3659 | 1/1   | 0.90 | 0.53 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1837 | 1/1   | 0.90 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 1N    | 203  | 1/1   | 0.90 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3415 | 1/1   | 0.90 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1697 | 1/1   | 0.90 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3720 | 1/1   | 0.90 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3558 | 1/1   | 0.90 | 0.10 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3406 | 1/1   | 0.90 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 2B    | 3004 | 1/1   | 0.90 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3077 | 1/1   | 0.90 | 0.41 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1845 | 1/1   | 0.90 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3666 | 1/1   | 0.90 | 0.10 | 20,20,20,20                 | 0     |
| 54  | MG   | 1a    | 1703 | 1/1   | 0.90 | 0.16 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3182 | 1/1   | 0.90 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3952 | 1/1   | 0.90 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3426 | 1/1   | 0.90 | 0.20 | 14,14,14,14                 | 0     |
| 54  | MG   | 2D    | 303  | 1/1   | 0.90 | 0.52 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3955 | 1/1   | 0.90 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 1d    | 304  | 1/1   | 0.90 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 2D    | 308  | 1/1   | 0.90 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | 2F    | 301  | 1/1   | 0.90 | 0.16 | 39,39,39,39                 | 0     |
| 54  | MG   | 2G    | 3002 | 1/1   | 0.90 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 1d    | 305  | 1/1   | 0.90 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3454 | 1/1   | 0.90 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3457 | 1/1   | 0.90 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 2Q    | 3001 | 1/1   | 0.90 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3462 | 1/1   | 0.90 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1718 | 1/1   | 0.90 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1l    | 103  | 1/1   | 0.90 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1726 | 1/1   | 0.90 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | 15    | 102  | 1/1   | 0.90 | 0.27 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3469 | 1/1   | 0.90 | 0.07 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3347 | 1/1   | 0.90 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3283 | 1/1   | 0.90 | 0.15 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3678 | 1/1   | 0.90 | 0.16 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3199 | 1/1   | 0.90 | 0.26 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3482 | 1/1   | 0.90 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3483 | 1/1   | 0.90 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3573 | 1/1   | 0.90 | 0.70 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1608 | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1744 | 1/1   | 0.90 | 0.26 | 62,62,62,62                 | 0     |
| 54  | MG   | 1y    | 3003 | 1/1   | 0.90 | 0.17 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3574 | 1/1   | 0.90 | 0.16 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3504 | 1/1   | 0.90 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3696 | 1/1   | 0.90 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1621 | 1/1   | 0.90 | 0.14 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1751 | 1/1   | 0.90 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3512 | 1/1   | 0.90 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3519 | 1/1   | 0.90 | 0.15 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3286 | 1/1   | 0.90 | 0.33 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3079 | 1/1   | 0.90 | 0.63 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3704 | 1/1   | 0.90 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3363 | 1/1   | 0.90 | 0.15 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3220 | 1/1   | 0.90 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3582 | 1/1   | 0.90 | 0.19 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1626 | 1/1   | 0.90 | 0.22 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3713 | 1/1   | 0.90 | 0.31 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3449 | 1/1   | 0.90 | 0.17 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3236 | 1/1   | 0.90 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3050 | 1/1   | 0.90 | 0.34 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3555 | 1/1   | 0.90 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 1661 | 1/1   | 0.90 | 0.41 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3244 | 1/1   | 0.90 | 1.30 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1778 | 1/1   | 0.90 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3250 | 1/1   | 0.90 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3058 | 1/1   | 0.90 | 0.21 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 1672 | 1/1   | 0.90 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1779 | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3063 | 1/1   | 0.90 | 0.47 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3065 | 1/1   | 0.90 | 0.41 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3301 | 1/1   | 0.90 | 0.20 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3256 | 1/1   | 0.90 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3085 | 1/1   | 0.90 | 0.09 | 36,36,36,36                 | 0     |
| 54  | MG   | 1B    | 217  | 1/1   | 0.90 | 0.37 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3597 | 1/1   | 0.90 | 0.32 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3610 | 1/1   | 0.90 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3290 | 1/1   | 0.90 | 0.15 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3607 | 1/1   | 0.90 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | 1B    | 221  | 1/1   | 0.90 | 0.18 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3391 | 1/1   | 0.90 | 0.23 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3613 | 1/1   | 0.90 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3088 | 1/1   | 0.90 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1B    | 225  | 1/1   | 0.90 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3615 | 1/1   | 0.90 | 0.18 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1B    | 230  | 1/1   | 0.90 | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 1720 | 1/1   | 0.90 | 0.18 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1806 | 1/1   | 0.90 | 0.20 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3317 | 1/1   | 0.90 | 0.11 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3105 | 1/1   | 0.90 | 0.49 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3751 | 1/1   | 0.90 | 0.31 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3644 | 1/1   | 0.90 | 0.15 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3109 | 1/1   | 0.90 | 0.49 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3021 | 1/1   | 0.90 | 0.25 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3656 | 1/1   | 0.90 | 0.21 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3004 | 1/1   | 0.90 | 0.23 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3070 | 1/1   | 0.90 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3123 | 1/1   | 0.90 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3102 | 1/1   | 0.90 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3928 | 1/1   | 0.90 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3671 | 1/1   | 0.90 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1818 | 1/1   | 0.90 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1819 | 1/1   | 0.90 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1673 | 1/1   | 0.90 | 0.35 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3143 | 1/1   | 0.90 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1772 | 1/1   | 0.91 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3660 | 1/1   | 0.91 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3661 | 1/1   | 0.91 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3079 | 1/1   | 0.91 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3666 | 1/1   | 0.91 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3946 | 1/1   | 0.91 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3328 | 1/1   | 0.91 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1605 | 1/1   | 0.91 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3084 | 1/1   | 0.91 | 0.25 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3508 | 1/1   | 0.91 | 0.14 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3513 | 1/1   | 0.91 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3092 | 1/1   | 0.91 | 0.41 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3682 | 1/1   | 0.91 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3514 | 1/1   | 0.91 | 0.20 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1613 | 1/1   | 0.91 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3321 | 1/1   | 0.91 | 0.14 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3358 | 1/1   | 0.91 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 1a    | 1618 | 1/1   | 0.91 | 0.29 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3369 | 1/1   | 0.91 | 0.27 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3786 | 1/1   | 0.91 | 0.16 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3373 | 1/1   | 0.91 | 0.16 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3374 | 1/1   | 0.91 | 0.10 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3522 | 1/1   | 0.91 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3717 | 1/1   | 0.91 | 0.27 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3379 | 1/1   | 0.91 | 0.16 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3213 | 1/1   | 0.91 | 0.20 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3051 | 1/1   | 0.91 | 0.60 | 26,26,26,26                 | 0     |
| 54  | MG   | 2B    | 3002 | 1/1   | 0.91 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | 1a    | 1625 | 1/1   | 0.91 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3260 | 1/1   | 0.91 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 2B    | 3008 | 1/1   | 0.91 | 0.08 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3411 | 1/1   | 0.91 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3532 | 1/1   | 0.91 | 0.17 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3667 | 1/1   | 0.91 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3217 | 1/1   | 0.91 | 0.61 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3543 | 1/1   | 0.91 | 0.24 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3548 | 1/1   | 0.91 | 0.15 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3831 | 1/1   | 0.91 | 0.13 | 19,19,19,19                 | 0     |
| 54  | MG   | 1a    | 1639 | 1/1   | 0.91 | 0.20 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 4013 | 1/1   | 0.91 | 0.86 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3413 | 1/1   | 0.91 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3677 | 1/1   | 0.91 | 0.28 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3833 | 1/1   | 0.91 | 0.12 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3425 | 1/1   | 0.91 | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3152 | 1/1   | 0.91 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | 2P    | 201  | 1/1   | 0.91 | 0.13 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1820 | 1/1   | 0.91 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3435 | 1/1   | 0.91 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3157 | 1/1   | 0.91 | 0.18 | 42,42,42,42                 | 0     |
| 54  | MG   | 2R    | 201  | 1/1   | 0.91 | 0.20 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3419 | 1/1   | 0.91 | 0.21 | 47,47,47,47                 | 0     |
| 54  | MG   | 1B    | 203  | 1/1   | 0.91 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3552 | 1/1   | 0.91 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1657 | 1/1   | 0.91 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 25    | 502  | 1/1   | 0.91 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3686 | 1/1   | 0.91 | 0.18 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3688 | 1/1   | 0.91 | 0.20 | 34,34,34,34                 | 0     |
| 54  | MG   | 1B    | 210  | 1/1   | 0.91 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3857 | 1/1   | 0.91 | 0.12 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3167 | 1/1   | 0.91 | 0.47 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1669 | 1/1   | 0.91 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3179 | 1/1   | 0.91 | 0.08 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3865 | 1/1   | 0.91 | 0.77 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3423 | 1/1   | 0.91 | 0.09 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3223 | 1/1   | 0.91 | 0.45 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3478 | 1/1   | 0.91 | 0.11 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3565 | 1/1   | 0.91 | 0.21 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3873 | 1/1   | 0.91 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 1617 | 1/1   | 0.91 | 0.19 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3229 | 1/1   | 0.91 | 0.24 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 1620 | 1/1   | 0.91 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1853 | 1/1   | 0.91 | 0.18 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3878 | 1/1   | 0.91 | 0.32 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3148 | 1/1   | 0.91 | 0.35 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3891 | 1/1   | 0.91 | 0.14 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3436 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3507 | 1/1   | 0.91 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 1635 | 1/1   | 0.91 | 0.15 | 71,71,71,71                 | 0     |
| 54  | MG   | 1a    | 1696 | 1/1   | 0.91 | 0.15 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3509 | 1/1   | 0.91 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | 1d    | 306  | 1/1   | 0.91 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3133 | 1/1   | 0.91 | 0.09 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3092 | 1/1   | 0.91 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3251 | 1/1   | 0.91 | 0.29 | 23,23,23,23                 | 0     |
| 54  | MG   | 1F    | 313  | 1/1   | 0.91 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3721 | 1/1   | 0.91 | 0.19 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3528 | 1/1   | 0.91 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3293 | 1/1   | 0.91 | 0.23 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3460 | 1/1   | 0.91 | 0.18 | 30,30,30,30                 | 0     |
| 54  | MG   | 1a    | 1709 | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3296 | 1/1   | 0.91 | 0.14 | 19,19,19,19                 | 0     |
| 54  | MG   | 2a    | 1666 | 1/1   | 0.91 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3140 | 1/1   | 0.91 | 0.46 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3183 | 1/1   | 0.91 | 0.15 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3551 | 1/1   | 0.91 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3005 | 1/1   | 0.91 | 0.27 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3224 | 1/1   | 0.91 | 0.63 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3554 | 1/1   | 0.91 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3225 | 1/1   | 0.91 | 0.21 | 56,56,56,56                 | 0     |
| 54  | MG   | 1O    | 8001 | 1/1   | 0.91 | 0.12 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3485 | 1/1   | 0.91 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 1P    | 203  | 1/1   | 0.91 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3929 | 1/1   | 0.91 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3573 | 1/1   | 0.91 | 0.16 | 19,19,19,19                 | 0     |
| 54  | MG   | 1a    | 1741 | 1/1   | 0.91 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3486 | 1/1   | 0.91 | 0.18 | 21,21,21,21                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3032 | 1/1   | 0.91 | 0.16 | 54,54,54,54                 | 0     |
| 54  | MG   | 1T    | 201  | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3249 | 1/1   | 0.91 | 0.14 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3302 | 1/1   | 0.91 | 0.16 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3043 | 1/1   | 0.91 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3493 | 1/1   | 0.91 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3598 | 1/1   | 0.91 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3051 | 1/1   | 0.91 | 0.18 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 1725 | 1/1   | 0.91 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3498 | 1/1   | 0.91 | 0.21 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3054 | 1/1   | 0.91 | 0.20 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3160 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3275 | 1/1   | 0.91 | 0.06 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 1743 | 1/1   | 0.91 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 1l    | 102  | 1/1   | 0.91 | 0.18 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3284 | 1/1   | 0.91 | 0.18 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1753 | 1/1   | 0.91 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3059 | 1/1   | 0.91 | 0.28 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3940 | 1/1   | 0.91 | 0.38 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3291 | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3766 | 1/1   | 0.91 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1759 | 1/1   | 0.91 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1761 | 1/1   | 0.91 | 0.07 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3070 | 1/1   | 0.91 | 0.59 | 42,42,42,42                 | 0     |
| 54  | MG   | 2r    | 8001 | 1/1   | 0.91 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MPD  | 1T    | 204  | 8/8   | 0.91 | 0.19 | 57,64,66,66                 | 0     |
| 57  | MPD  | 1a    | 1854 | 8/8   | 0.91 | 0.15 | 46,63,67,69                 | 0     |
| 54  | MG   | 1A    | 3311 | 1/1   | 0.91 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3944 | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3075 | 1/1   | 0.91 | 0.68 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3077 | 1/1   | 0.91 | 0.17 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3281 | 1/1   | 0.92 | 0.18 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3283 | 1/1   | 0.92 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3047 | 1/1   | 0.92 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1739 | 1/1   | 0.92 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3083 | 1/1   | 0.92 | 0.26 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3315 | 1/1   | 0.92 | 0.12 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3036 | 1/1   | 0.92 | 0.18 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3657 | 1/1   | 0.92 | 0.17 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3293 | 1/1   | 0.92 | 0.15 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3294 | 1/1   | 0.92 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3900 | 1/1   | 0.92 | 0.19 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3428 | 1/1   | 0.92 | 0.31 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3322 | 1/1   | 0.92 | 0.17 | 21,21,21,21                 | 0     |
| 54  | MG   | 1R    | 201  | 1/1   | 0.92 | 0.36 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3714 | 1/1   | 0.92 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3038 | 1/1   | 0.92 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3257 | 1/1   | 0.92 | 0.31 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3437 | 1/1   | 0.92 | 0.20 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1756 | 1/1   | 0.92 | 0.15 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3674 | 1/1   | 0.92 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3197 | 1/1   | 0.92 | 0.14 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3323 | 1/1   | 0.92 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3677 | 1/1   | 0.92 | 0.30 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3680 | 1/1   | 0.92 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3924 | 1/1   | 0.92 | 0.16 | 45,45,45,45                 | 0     |
| 54  | MG   | 10    | 103  | 1/1   | 0.92 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3732 | 1/1   | 0.92 | 0.25 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1768 | 1/1   | 0.92 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | 10    | 106  | 1/1   | 0.92 | 0.39 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3203 | 1/1   | 0.92 | 0.24 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3339 | 1/1   | 0.92 | 0.10 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3446 | 1/1   | 0.92 | 0.22 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3932 | 1/1   | 0.92 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3933 | 1/1   | 0.92 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3702 | 1/1   | 0.92 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3739 | 1/1   | 0.92 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3094 | 1/1   | 0.92 | 0.23 | 49,49,49,49                 | 0     |
| 54  | MG   | 19    | 503  | 1/1   | 0.92 | 0.16 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3337 | 1/1   | 0.92 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3075 | 1/1   | 0.92 | 0.39 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3371 | 1/1   | 0.92 | 0.17 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3341 | 1/1   | 0.92 | 0.13 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3261 | 1/1   | 0.92 | 0.44 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1788 | 1/1   | 0.92 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3108 | 1/1   | 0.92 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | 2B    | 3011 | 1/1   | 0.92 | 0.08 | 65,65,65,65                 | 0     |
| 54  | MG   | 2B    | 3012 | 1/1   | 0.92 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3939 | 1/1   | 0.92 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3263 | 1/1   | 0.92 | 0.39 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3266 | 1/1   | 0.92 | 0.66 | 40,40,40,40                 | 0     |
| 54  | MG   | 2B    | 3017 | 1/1   | 0.92 | 0.13 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3114 | 1/1   | 0.92 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | 2B    | 3019 | 1/1   | 0.92 | 0.09 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3605 | 1/1   | 0.92 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 2D    | 302  | 1/1   | 0.92 | 0.91 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3608 | 1/1   | 0.92 | 0.18 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1803 | 1/1   | 0.92 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3765 | 1/1   | 0.92 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3132 | 1/1   | 0.92 | 0.14 | 43,43,43,43                 | 0     |
| 54  | MG   | 2E    | 302  | 1/1   | 0.92 | 0.39 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3402 | 1/1   | 0.92 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 2F    | 303  | 1/1   | 0.92 | 0.70 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3353 | 1/1   | 0.92 | 0.13 | 18,18,18,18                 | 0     |
| 54  | MG   | 2A    | 3136 | 1/1   | 0.92 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3767 | 1/1   | 0.92 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3139 | 1/1   | 0.92 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3773 | 1/1   | 0.92 | 0.17 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3419 | 1/1   | 0.92 | 0.20 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1812 | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3125 | 1/1   | 0.92 | 0.46 | 30,30,30,30                 | 0     |
| 54  | MG   | 2T    | 3001 | 1/1   | 0.92 | 0.24 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3780 | 1/1   | 0.92 | 0.21 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3426 | 1/1   | 0.92 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3613 | 1/1   | 0.92 | 0.26 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3163 | 1/1   | 0.92 | 0.25 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3151 | 1/1   | 0.92 | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | 28    | 8001 | 1/1   | 0.92 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3210 | 1/1   | 0.92 | 0.32 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3153 | 1/1   | 0.92 | 0.47 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3154 | 1/1   | 0.92 | 0.19 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3212 | 1/1   | 0.92 | 0.57 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3453 | 1/1   | 0.92 | 0.31 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1634 | 1/1   | 0.92 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3456 | 1/1   | 0.92 | 0.14 | 31,31,31,31                 | 0     |
| 54  | MG   | 2a    | 1606 | 1/1   | 0.92 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1821 | 1/1   | 0.92 | 0.18 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3460 | 1/1   | 0.92 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3164 | 1/1   | 0.92 | 0.11 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3632 | 1/1   | 0.92 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3465 | 1/1   | 0.92 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3008 | 1/1   | 0.92 | 0.10 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3966 | 1/1   | 0.92 | 0.43 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3281 | 1/1   | 0.92 | 0.23 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3981 | 1/1   | 0.92 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3797 | 1/1   | 0.92 | 0.33 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3641 | 1/1   | 0.92 | 0.19 | 29,29,29,29                 | 0     |
| 54  | MG   | 2a    | 1626 | 1/1   | 0.92 | 0.21 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1836 | 1/1   | 0.92 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 4005 | 1/1   | 0.92 | 0.31 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1839 | 1/1   | 0.92 | 0.08 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3172 | 1/1   | 0.92 | 0.86 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3512 | 1/1   | 0.92 | 0.19 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3651 | 1/1   | 0.92 | 0.30 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3186 | 1/1   | 0.92 | 0.19 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3809 | 1/1   | 0.92 | 0.23 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3501 | 1/1   | 0.92 | 0.14 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3132 | 1/1   | 0.92 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3503 | 1/1   | 0.92 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1664 | 1/1   | 0.92 | 0.21 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3506 | 1/1   | 0.92 | 0.10 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 1650 | 1/1   | 0.92 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 4027 | 1/1   | 0.92 | 0.48 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 1655 | 1/1   | 0.92 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3655 | 1/1   | 0.92 | 0.36 | 30,30,30,30                 | 0     |
| 54  | MG   | 2a    | 1658 | 1/1   | 0.92 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3818 | 1/1   | 0.92 | 0.17 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3058 | 1/1   | 0.92 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1856 | 1/1   | 0.92 | 0.19 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 1664 | 1/1   | 0.92 | 0.11 | 61,61,61,61                 | 0     |
| 54  | MG   | 1b    | 3001 | 1/1   | 0.92 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3823 | 1/1   | 0.92 | 0.30 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3660 | 1/1   | 0.92 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 1B    | 208  | 1/1   | 0.92 | 0.24 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3392 | 1/1   | 0.92 | 0.22 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3521 | 1/1   | 0.92 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | 1B    | 215  | 1/1   | 0.92 | 0.28 | 61,61,61,61                 | 0     |
| 54  | MG   | 1e    | 3002 | 1/1   | 0.92 | 0.41 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3207 | 1/1   | 0.92 | 0.35 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3208 | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3211 | 1/1   | 0.92 | 0.48 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3549 | 1/1   | 0.92 | 0.20 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3292 | 1/1   | 0.92 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 1h    | 3001 | 1/1   | 0.92 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3061 | 1/1   | 0.92 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3116 | 1/1   | 0.92 | 0.23 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1689 | 1/1   | 0.92 | 0.18 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3558 | 1/1   | 0.92 | 0.09 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1691 | 1/1   | 0.92 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 1B    | 222  | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 1707 | 1/1   | 0.92 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3566 | 1/1   | 0.92 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3837 | 1/1   | 0.92 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3142 | 1/1   | 0.92 | 0.21 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3848 | 1/1   | 0.92 | 0.14 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3403 | 1/1   | 0.92 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3674 | 1/1   | 0.92 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3235 | 1/1   | 0.92 | 0.15 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3118 | 1/1   | 0.92 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3012 | 1/1   | 0.92 | 0.16 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3408 | 1/1   | 0.92 | 0.19 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3538 | 1/1   | 0.92 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3539 | 1/1   | 0.92 | 0.14 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3147 | 1/1   | 0.92 | 0.20 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3413 | 1/1   | 0.92 | 0.29 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3031 | 1/1   | 0.92 | 0.19 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3549 | 1/1   | 0.92 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3261 | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3609 | 1/1   | 0.92 | 0.18 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3119 | 1/1   | 0.92 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3265 | 1/1   | 0.92 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3614 | 1/1   | 0.92 | 0.17 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3268 | 1/1   | 0.92 | 0.10 | 29,29,29,29                 | 0     |
| 54  | MG   | 1a    | 1730 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3882 | 1/1   | 0.92 | 0.04 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3310 | 1/1   | 0.92 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3046 | 1/1   | 0.92 | 0.23 | 59,59,59,59                 | 0     |
| 54  | MG   | 1E    | 306  | 1/1   | 0.93 | 0.13 | 31,31,31,31                 | 0     |
| 54  | MG   | 1F    | 302  | 1/1   | 0.93 | 0.13 | 32,32,32,32                 | 0     |
| 54  | MG   | 1F    | 307  | 1/1   | 0.93 | 0.37 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3624 | 1/1   | 0.93 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3883 | 1/1   | 0.93 | 0.56 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3630 | 1/1   | 0.93 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3048 | 1/1   | 0.93 | 0.20 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3049 | 1/1   | 0.93 | 0.18 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3050 | 1/1   | 0.93 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1738 | 1/1   | 0.93 | 0.30 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3884 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3646 | 1/1   | 0.93 | 0.25 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3647 | 1/1   | 0.93 | 0.17 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1A    | 3728 | 1/1   | 0.93 | 0.22 | 38,38,38,38                | 0     |
| 54  | MG   | 1A    | 3188 | 1/1   | 0.93 | 0.18 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3335 | 1/1   | 0.93 | 0.15 | 22,22,22,22                | 0     |
| 54  | MG   | 1A    | 3733 | 1/1   | 0.93 | 0.12 | 42,42,42,42                | 0     |
| 54  | MG   | 1a    | 1747 | 1/1   | 0.93 | 0.20 | 56,56,56,56                | 0     |
| 54  | MG   | 1A    | 3174 | 1/1   | 0.93 | 0.34 | 34,34,34,34                | 0     |
| 54  | MG   | 1A    | 3175 | 1/1   | 0.93 | 0.56 | 35,35,35,35                | 0     |
| 54  | MG   | 1A    | 3902 | 1/1   | 0.93 | 0.14 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3503 | 1/1   | 0.93 | 0.13 | 58,58,58,58                | 0     |
| 54  | MG   | 2A    | 3663 | 1/1   | 0.93 | 0.09 | 61,61,61,61                | 0     |
| 54  | MG   | 2A    | 3664 | 1/1   | 0.93 | 0.09 | 57,57,57,57                | 0     |
| 54  | MG   | 1A    | 3904 | 1/1   | 0.93 | 0.13 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3127 | 1/1   | 0.93 | 0.18 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3668 | 1/1   | 0.93 | 0.10 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3218 | 1/1   | 0.93 | 0.44 | 30,30,30,30                | 0     |
| 54  | MG   | 1A    | 3343 | 1/1   | 0.93 | 0.14 | 56,56,56,56                | 0     |
| 54  | MG   | 2A    | 3076 | 1/1   | 0.93 | 0.33 | 44,44,44,44                | 0     |
| 54  | MG   | 1a    | 1757 | 1/1   | 0.93 | 0.11 | 77,77,77,77                | 0     |
| 54  | MG   | 1A    | 3417 | 1/1   | 0.93 | 0.16 | 20,20,20,20                | 0     |
| 54  | MG   | 1A    | 3178 | 1/1   | 0.93 | 0.29 | 29,29,29,29                | 0     |
| 54  | MG   | 1T    | 203  | 1/1   | 0.93 | 0.14 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3753 | 1/1   | 0.93 | 0.14 | 35,35,35,35                | 0     |
| 54  | MG   | 2A    | 3083 | 1/1   | 0.93 | 0.17 | 49,49,49,49                | 0     |
| 54  | MG   | 1A    | 3621 | 1/1   | 0.93 | 0.10 | 52,52,52,52                | 0     |
| 54  | MG   | 1a    | 1771 | 1/1   | 0.93 | 0.16 | 46,46,46,46                | 0     |
| 54  | MG   | 2A    | 3343 | 1/1   | 0.93 | 0.22 | 50,50,50,50                | 0     |
| 54  | MG   | 1V    | 203  | 1/1   | 0.93 | 0.20 | 55,55,55,55                | 0     |
| 54  | MG   | 2A    | 3349 | 1/1   | 0.93 | 0.17 | 56,56,56,56                | 0     |
| 54  | MG   | 1A    | 3520 | 1/1   | 0.93 | 0.14 | 38,38,38,38                | 0     |
| 54  | MG   | 1Z    | 8001 | 1/1   | 0.93 | 0.19 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3196 | 1/1   | 0.93 | 0.57 | 40,40,40,40                | 0     |
| 54  | MG   | 2A    | 3361 | 1/1   | 0.93 | 0.11 | 33,33,33,33                | 0     |
| 54  | MG   | 2A    | 3362 | 1/1   | 0.93 | 0.14 | 34,34,34,34                | 0     |
| 54  | MG   | 2A    | 3363 | 1/1   | 0.93 | 0.16 | 61,61,61,61                | 0     |
| 54  | MG   | 1A    | 3760 | 1/1   | 0.93 | 0.24 | 61,61,61,61                | 0     |
| 54  | MG   | 1A    | 3761 | 1/1   | 0.93 | 0.13 | 32,32,32,32                | 0     |
| 54  | MG   | 1A    | 3349 | 1/1   | 0.93 | 0.15 | 40,40,40,40                | 0     |
| 54  | MG   | 1A    | 3425 | 1/1   | 0.93 | 0.13 | 35,35,35,35                | 0     |
| 54  | MG   | 2A    | 3724 | 1/1   | 0.93 | 0.42 | 32,32,32,32                | 0     |
| 54  | MG   | 1A    | 3300 | 1/1   | 0.93 | 0.14 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3768 | 1/1   | 0.93 | 0.11 | 54,54,54,54                | 0     |
| 54  | MG   | 2B    | 3003 | 1/1   | 0.93 | 0.09 | 74,74,74,74                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3646 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 2B    | 3005 | 1/1   | 0.93 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3377 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1786 | 1/1   | 0.93 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3381 | 1/1   | 0.93 | 0.13 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3383 | 1/1   | 0.93 | 0.23 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3427 | 1/1   | 0.93 | 0.13 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3113 | 1/1   | 0.93 | 0.27 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3180 | 1/1   | 0.93 | 0.42 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3388 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3265 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3942 | 1/1   | 0.93 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3156 | 1/1   | 0.93 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3535 | 1/1   | 0.93 | 0.26 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3131 | 1/1   | 0.93 | 0.83 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3305 | 1/1   | 0.93 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3367 | 1/1   | 0.93 | 0.18 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3235 | 1/1   | 0.93 | 0.39 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3442 | 1/1   | 0.93 | 0.15 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3376 | 1/1   | 0.93 | 0.12 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3272 | 1/1   | 0.93 | 0.16 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3954 | 1/1   | 0.93 | 0.09 | 36,36,36,36                 | 0     |
| 54  | MG   | 2G    | 3001 | 1/1   | 0.93 | 0.08 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3417 | 1/1   | 0.93 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3144 | 1/1   | 0.93 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3551 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3800 | 1/1   | 0.93 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3238 | 1/1   | 0.93 | 0.56 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3960 | 1/1   | 0.93 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3673 | 1/1   | 0.93 | 0.17 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3320 | 1/1   | 0.93 | 0.10 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3432 | 1/1   | 0.93 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3434 | 1/1   | 0.93 | 0.13 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3963 | 1/1   | 0.93 | 0.25 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3436 | 1/1   | 0.93 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3439 | 1/1   | 0.93 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3444 | 1/1   | 0.93 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3446 | 1/1   | 0.93 | 0.13 | 30,30,30,30                 | 0     |
| 54  | MG   | 1a    | 1822 | 1/1   | 0.93 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3452 | 1/1   | 0.93 | 0.15 | 21,21,21,21                 | 0     |
| 54  | MG   | 1a    | 1825 | 1/1   | 0.93 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3159 | 1/1   | 0.93 | 0.12 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1A    | 3815 | 1/1   | 0.93 | 0.10 | 33,33,33,33                | 0     |
| 54  | MG   | 2A    | 3161 | 1/1   | 0.93 | 0.17 | 46,46,46,46                | 0     |
| 54  | MG   | 1A    | 3968 | 1/1   | 0.93 | 0.10 | 11,11,11,11                | 0     |
| 54  | MG   | 1a    | 1831 | 1/1   | 0.93 | 0.10 | 54,54,54,54                | 0     |
| 54  | MG   | 2A    | 3459 | 1/1   | 0.93 | 0.11 | 38,38,38,38                | 0     |
| 54  | MG   | 1A    | 3562 | 1/1   | 0.93 | 0.07 | 32,32,32,32                | 0     |
| 54  | MG   | 1A    | 3457 | 1/1   | 0.93 | 0.09 | 64,64,64,64                | 0     |
| 54  | MG   | 1A    | 3387 | 1/1   | 0.93 | 0.08 | 54,54,54,54                | 0     |
| 54  | MG   | 1a    | 1648 | 1/1   | 0.93 | 0.07 | 72,72,72,72                | 0     |
| 54  | MG   | 1A    | 3463 | 1/1   | 0.93 | 0.13 | 19,19,19,19                | 0     |
| 54  | MG   | 1A    | 3995 | 1/1   | 0.93 | 0.20 | 26,26,26,26                | 0     |
| 54  | MG   | 2A    | 3174 | 1/1   | 0.93 | 0.23 | 45,45,45,45                | 0     |
| 54  | MG   | 1a    | 1651 | 1/1   | 0.93 | 0.25 | 59,59,59,59                | 0     |
| 54  | MG   | 2A    | 3471 | 1/1   | 0.93 | 0.10 | 61,61,61,61                | 0     |
| 54  | MG   | 1A    | 4000 | 1/1   | 0.93 | 0.11 | 30,30,30,30                | 0     |
| 54  | MG   | 2a    | 1624 | 1/1   | 0.93 | 0.15 | 65,65,65,65                | 0     |
| 54  | MG   | 2a    | 1625 | 1/1   | 0.93 | 0.13 | 67,67,67,67                | 0     |
| 54  | MG   | 1A    | 3687 | 1/1   | 0.93 | 0.10 | 44,44,44,44                | 0     |
| 54  | MG   | 1a    | 1655 | 1/1   | 0.93 | 0.26 | 57,57,57,57                | 0     |
| 54  | MG   | 1A    | 3826 | 1/1   | 0.93 | 0.19 | 26,26,26,26                | 0     |
| 54  | MG   | 2A    | 3479 | 1/1   | 0.93 | 0.14 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 3829 | 1/1   | 0.93 | 0.15 | 54,54,54,54                | 0     |
| 54  | MG   | 1A    | 3570 | 1/1   | 0.93 | 0.25 | 47,47,47,47                | 0     |
| 54  | MG   | 2a    | 1637 | 1/1   | 0.93 | 0.19 | 63,63,63,63                | 0     |
| 54  | MG   | 1a    | 1660 | 1/1   | 0.93 | 0.18 | 46,46,46,46                | 0     |
| 54  | MG   | 1a    | 1848 | 1/1   | 0.93 | 0.21 | 53,53,53,53                | 0     |
| 54  | MG   | 2a    | 1640 | 1/1   | 0.93 | 0.17 | 53,53,53,53                | 0     |
| 54  | MG   | 2A    | 3190 | 1/1   | 0.93 | 0.12 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 4016 | 1/1   | 0.93 | 0.48 | 41,41,41,41                | 0     |
| 54  | MG   | 2A    | 3500 | 1/1   | 0.93 | 0.12 | 51,51,51,51                | 0     |
| 54  | MG   | 1A    | 3471 | 1/1   | 0.93 | 0.10 | 31,31,31,31                | 0     |
| 54  | MG   | 1a    | 1665 | 1/1   | 0.93 | 0.13 | 59,59,59,59                | 0     |
| 54  | MG   | 1a    | 1666 | 1/1   | 0.93 | 0.55 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 4022 | 1/1   | 0.93 | 0.15 | 30,30,30,30                | 0     |
| 54  | MG   | 1A    | 3166 | 1/1   | 0.93 | 0.10 | 32,32,32,32                | 0     |
| 54  | MG   | 2a    | 1653 | 1/1   | 0.93 | 0.10 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3700 | 1/1   | 0.93 | 0.08 | 34,34,34,34                | 0     |
| 54  | MG   | 1A    | 3701 | 1/1   | 0.93 | 0.19 | 29,29,29,29                | 0     |
| 54  | MG   | 1A    | 3475 | 1/1   | 0.93 | 0.14 | 42,42,42,42                | 0     |
| 54  | MG   | 1A    | 3841 | 1/1   | 0.93 | 0.15 | 29,29,29,29                | 0     |
| 54  | MG   | 2A    | 3201 | 1/1   | 0.93 | 0.33 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3101 | 1/1   | 0.93 | 0.39 | 30,30,30,30                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3481 | 1/1   | 0.93 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3106 | 1/1   | 0.93 | 0.42 | 40,40,40,40                 | 0     |
| 54  | MG   | 1g    | 3001 | 1/1   | 0.93 | 0.29 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3707 | 1/1   | 0.93 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 1670 | 1/1   | 0.93 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3532 | 1/1   | 0.93 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3533 | 1/1   | 0.93 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3534 | 1/1   | 0.93 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3579 | 1/1   | 0.93 | 0.20 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3861 | 1/1   | 0.93 | 0.17 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3212 | 1/1   | 0.93 | 0.38 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3213 | 1/1   | 0.93 | 0.13 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3864 | 1/1   | 0.93 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | 1B    | 218  | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3712 | 1/1   | 0.93 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3217 | 1/1   | 0.93 | 0.16 | 43,43,43,43                 | 0     |
| 54  | MG   | 2a    | 1688 | 1/1   | 0.93 | 0.19 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1692 | 1/1   | 0.93 | 0.21 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3395 | 1/1   | 0.93 | 0.12 | 13,13,13,13                 | 0     |
| 54  | MG   | 1A    | 3583 | 1/1   | 0.93 | 0.22 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3868 | 1/1   | 0.93 | 0.20 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3001 | 1/1   | 0.93 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3004 | 1/1   | 0.93 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3717 | 1/1   | 0.93 | 0.41 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3872 | 1/1   | 0.93 | 0.16 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3141 | 1/1   | 0.93 | 0.19 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3234 | 1/1   | 0.93 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1721 | 1/1   | 0.93 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3570 | 1/1   | 0.93 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3487 | 1/1   | 0.93 | 0.46 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1705 | 1/1   | 0.93 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 1735 | 1/1   | 0.93 | 0.17 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3238 | 1/1   | 0.93 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 1740 | 1/1   | 0.93 | 0.26 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3582 | 1/1   | 0.93 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3586 | 1/1   | 0.93 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | 2A    | 3017 | 1/1   | 0.93 | 0.67 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3877 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3282 | 1/1   | 0.93 | 0.36 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3247 | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3022 | 1/1   | 0.93 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 1751 | 1/1   | 0.93 | 0.11 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3023 | 1/1   | 0.93 | 0.26 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1714 | 1/1   | 0.93 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3881 | 1/1   | 0.93 | 0.21 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3600 | 1/1   | 0.93 | 0.28 | 54,54,54,54                 | 0     |
| 54  | MG   | 1D    | 311  | 1/1   | 0.93 | 0.19 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3034 | 1/1   | 0.93 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MPD  | 1A    | 3988 | 8/8   | 0.93 | 0.21 | 48,52,54,59                 | 0     |
| 54  | MG   | 1E    | 301  | 1/1   | 0.93 | 0.16 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3039 | 1/1   | 0.93 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3040 | 1/1   | 0.93 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MPD  | 2A    | 3711 | 8/8   | 0.93 | 0.12 | 48,60,64,64                 | 0     |
| 54  | MG   | 2A    | 3612 | 1/1   | 0.93 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3269 | 1/1   | 0.93 | 0.15 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3724 | 1/1   | 0.93 | 0.15 | 27,27,27,27                 | 0     |
| 59  | ZN   | 24    | 501  | 1/1   | 0.93 | 0.05 | 108,108,108,108             | 0     |
| 54  | MG   | 1A    | 3664 | 1/1   | 0.94 | 0.20 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3591 | 1/1   | 0.94 | 0.26 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3233 | 1/1   | 0.94 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 1g    | 3002 | 1/1   | 0.94 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3595 | 1/1   | 0.94 | 0.21 | 53,53,53,53                 | 0     |
| 54  | MG   | 1g    | 3003 | 1/1   | 0.94 | 0.15 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3542 | 1/1   | 0.94 | 0.23 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3983 | 1/1   | 0.94 | 0.30 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3239 | 1/1   | 0.94 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3601 | 1/1   | 0.94 | 0.31 | 57,57,57,57                 | 0     |
| 54  | MG   | 1l    | 3001 | 1/1   | 0.94 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3606 | 1/1   | 0.94 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3198 | 1/1   | 0.94 | 0.49 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3811 | 1/1   | 0.94 | 0.22 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3998 | 1/1   | 0.94 | 0.52 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3544 | 1/1   | 0.94 | 0.55 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3611 | 1/1   | 0.94 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 4003 | 1/1   | 0.94 | 0.18 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3816 | 1/1   | 0.94 | 0.13 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3669 | 1/1   | 0.94 | 0.16 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 4008 | 1/1   | 0.94 | 0.29 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 4009 | 1/1   | 0.94 | 0.69 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3545 | 1/1   | 0.94 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 4012 | 1/1   | 0.94 | 0.50 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3626 | 1/1   | 0.94 | 0.06 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3627 | 1/1   | 0.94 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3819 | 1/1   | 0.94 | 0.09 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1675 | 1/1   | 0.94 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3631 | 1/1   | 0.94 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3201 | 1/1   | 0.94 | 0.51 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3821 | 1/1   | 0.94 | 0.14 | 26,26,26,26                 | 0     |
| 54  | MG   | 1a    | 1678 | 1/1   | 0.94 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3636 | 1/1   | 0.94 | 0.24 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3639 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3137 | 1/1   | 0.94 | 0.14 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3642 | 1/1   | 0.94 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3453 | 1/1   | 0.94 | 0.07 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3108 | 1/1   | 0.94 | 0.45 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3139 | 1/1   | 0.94 | 0.23 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3028 | 1/1   | 0.94 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3649 | 1/1   | 0.94 | 0.23 | 38,38,38,38                 | 0     |
| 54  | MG   | 1a    | 1685 | 1/1   | 0.94 | 0.29 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3652 | 1/1   | 0.94 | 0.20 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3654 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3461 | 1/1   | 0.94 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1687 | 1/1   | 0.94 | 0.22 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1688 | 1/1   | 0.94 | 0.20 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3388 | 1/1   | 0.94 | 0.18 | 22,22,22,22                 | 0     |
| 54  | MG   | 1a    | 1690 | 1/1   | 0.94 | 0.17 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3297 | 1/1   | 0.94 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3298 | 1/1   | 0.94 | 0.16 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3680 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3681 | 1/1   | 0.94 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3665 | 1/1   | 0.94 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3560 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 1B    | 209  | 1/1   | 0.94 | 0.09 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3306 | 1/1   | 0.94 | 0.13 | 27,27,27,27                 | 0     |
| 54  | MG   | 1a    | 1698 | 1/1   | 0.94 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3670 | 1/1   | 0.94 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3309 | 1/1   | 0.94 | 0.14 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3469 | 1/1   | 0.94 | 0.09 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3315 | 1/1   | 0.94 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3390 | 1/1   | 0.94 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3112 | 1/1   | 0.94 | 0.48 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3320 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3691 | 1/1   | 0.94 | 0.18 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3679 | 1/1   | 0.94 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3850 | 1/1   | 0.94 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3052 | 1/1   | 0.94 | 0.22 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1A    | 3693 | 1/1   | 0.94 | 0.10 | 33,33,33,33                | 0     |
| 54  | MG   | 2A    | 3329 | 1/1   | 0.94 | 0.20 | 29,29,29,29                | 0     |
| 54  | MG   | 1A    | 3313 | 1/1   | 0.94 | 0.10 | 46,46,46,46                | 0     |
| 54  | MG   | 1A    | 3697 | 1/1   | 0.94 | 0.21 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3690 | 1/1   | 0.94 | 0.07 | 67,67,67,67                | 0     |
| 54  | MG   | 1a    | 1711 | 1/1   | 0.94 | 0.21 | 58,58,58,58                | 0     |
| 54  | MG   | 2A    | 3336 | 1/1   | 0.94 | 0.15 | 36,36,36,36                | 0     |
| 54  | MG   | 2A    | 3693 | 1/1   | 0.94 | 0.10 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3859 | 1/1   | 0.94 | 0.14 | 16,16,16,16                | 0     |
| 54  | MG   | 1A    | 3476 | 1/1   | 0.94 | 0.17 | 14,14,14,14                | 0     |
| 54  | MG   | 1B    | 226  | 1/1   | 0.94 | 0.13 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3698 | 1/1   | 0.94 | 0.36 | 40,40,40,40                | 0     |
| 54  | MG   | 2A    | 3700 | 1/1   | 0.94 | 0.15 | 21,21,21,21                | 0     |
| 54  | MG   | 1a    | 1719 | 1/1   | 0.94 | 0.13 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3862 | 1/1   | 0.94 | 0.18 | 33,33,33,33                | 0     |
| 54  | MG   | 2A    | 3705 | 1/1   | 0.94 | 0.88 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3706 | 1/1   | 0.94 | 0.21 | 48,48,48,48                | 0     |
| 54  | MG   | 2A    | 3707 | 1/1   | 0.94 | 0.18 | 61,61,61,61                | 0     |
| 54  | MG   | 2A    | 3712 | 1/1   | 0.94 | 0.39 | 41,41,41,41                | 0     |
| 54  | MG   | 2A    | 3715 | 1/1   | 0.94 | 0.77 | 37,37,37,37                | 0     |
| 54  | MG   | 1a    | 1723 | 1/1   | 0.94 | 0.14 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3719 | 1/1   | 0.94 | 0.23 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3026 | 1/1   | 0.94 | 0.41 | 28,28,28,28                | 0     |
| 54  | MG   | 1a    | 1727 | 1/1   | 0.94 | 0.20 | 43,43,43,43                | 0     |
| 54  | MG   | 2A    | 3723 | 1/1   | 0.94 | 0.58 | 37,37,37,37                | 0     |
| 54  | MG   | 1A    | 3057 | 1/1   | 0.94 | 0.25 | 27,27,27,27                | 0     |
| 54  | MG   | 2A    | 3073 | 1/1   | 0.94 | 0.12 | 45,45,45,45                | 0     |
| 54  | MG   | 1D    | 303  | 1/1   | 0.94 | 0.20 | 44,44,44,44                | 0     |
| 54  | MG   | 1A    | 3483 | 1/1   | 0.94 | 0.17 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3367 | 1/1   | 0.94 | 0.12 | 47,47,47,47                | 0     |
| 54  | MG   | 1a    | 1734 | 1/1   | 0.94 | 0.16 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3397 | 1/1   | 0.94 | 0.14 | 49,49,49,49                | 0     |
| 54  | MG   | 1A    | 3014 | 1/1   | 0.94 | 0.39 | 44,44,44,44                | 0     |
| 54  | MG   | 1A    | 3706 | 1/1   | 0.94 | 0.10 | 32,32,32,32                | 0     |
| 54  | MG   | 2A    | 3372 | 1/1   | 0.94 | 0.10 | 51,51,51,51                | 0     |
| 54  | MG   | 1a    | 1740 | 1/1   | 0.94 | 0.09 | 59,59,59,59                | 0     |
| 54  | MG   | 1D    | 313  | 1/1   | 0.94 | 0.28 | 43,43,43,43                | 0     |
| 54  | MG   | 1A    | 3871 | 1/1   | 0.94 | 0.24 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3059 | 1/1   | 0.94 | 0.12 | 42,42,42,42                | 0     |
| 54  | MG   | 1A    | 3400 | 1/1   | 0.94 | 0.15 | 35,35,35,35                | 0     |
| 54  | MG   | 1a    | 1746 | 1/1   | 0.94 | 0.07 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3382 | 1/1   | 0.94 | 0.10 | 43,43,43,43                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3093 | 1/1   | 0.94 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3711 | 1/1   | 0.94 | 0.20 | 30,30,30,30                 | 0     |
| 54  | MG   | 1F    | 306  | 1/1   | 0.94 | 0.16 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3876 | 1/1   | 0.94 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | 1F    | 309  | 1/1   | 0.94 | 0.24 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3101 | 1/1   | 0.94 | 0.21 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3392 | 1/1   | 0.94 | 0.18 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3581 | 1/1   | 0.94 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3121 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1F    | 312  | 1/1   | 0.94 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3091 | 1/1   | 0.94 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3496 | 1/1   | 0.94 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3589 | 1/1   | 0.94 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | 2N    | 8001 | 1/1   | 0.94 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3590 | 1/1   | 0.94 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3591 | 1/1   | 0.94 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 1H    | 8002 | 1/1   | 0.94 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3115 | 1/1   | 0.94 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 1N    | 201  | 1/1   | 0.94 | 0.32 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3414 | 1/1   | 0.94 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 2W    | 8001 | 1/1   | 0.94 | 0.33 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3118 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3120 | 1/1   | 0.94 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3122 | 1/1   | 0.94 | 0.20 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3422 | 1/1   | 0.94 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3060 | 1/1   | 0.94 | 0.20 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3726 | 1/1   | 0.94 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3898 | 1/1   | 0.94 | 0.08 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3127 | 1/1   | 0.94 | 0.26 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3429 | 1/1   | 0.94 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3727 | 1/1   | 0.94 | 0.25 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3431 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3019 | 1/1   | 0.94 | 0.44 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3598 | 1/1   | 0.94 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG   | 1R    | 202  | 1/1   | 0.94 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3599 | 1/1   | 0.94 | 0.24 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3138 | 1/1   | 0.94 | 0.13 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3441 | 1/1   | 0.94 | 0.27 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 1612 | 1/1   | 0.94 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3443 | 1/1   | 0.94 | 0.16 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3226 | 1/1   | 0.94 | 0.35 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3140 | 1/1   | 0.94 | 0.15 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 1616 | 1/1   | 0.94 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3501 | 1/1   | 0.94 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 1T    | 202  | 1/1   | 0.94 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3905 | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3604 | 1/1   | 0.94 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2a    | 1622 | 1/1   | 0.94 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1785 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3067 | 1/1   | 0.94 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3606 | 1/1   | 0.94 | 0.33 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1789 | 1/1   | 0.94 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3458 | 1/1   | 0.94 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG   | 1W    | 3001 | 1/1   | 0.94 | 0.22 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3504 | 1/1   | 0.94 | 0.11 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3609 | 1/1   | 0.94 | 0.37 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1796 | 1/1   | 0.94 | 0.24 | 50,50,50,50                 | 0     |
| 54  | MG   | 10    | 101  | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1799 | 1/1   | 0.94 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1800 | 1/1   | 0.94 | 0.23 | 43,43,43,43                 | 0     |
| 54  | MG   | 10    | 102  | 1/1   | 0.94 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3163 | 1/1   | 0.94 | 0.28 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3506 | 1/1   | 0.94 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | 10    | 104  | 1/1   | 0.94 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3475 | 1/1   | 0.94 | 0.18 | 30,30,30,30                 | 0     |
| 54  | MG   | 2a    | 1647 | 1/1   | 0.94 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3048 | 1/1   | 0.94 | 0.30 | 33,33,33,33                 | 0     |
| 54  | MG   | 1a    | 1807 | 1/1   | 0.94 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3128 | 1/1   | 0.94 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3236 | 1/1   | 0.94 | 0.73 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3162 | 1/1   | 0.94 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 2a    | 1654 | 1/1   | 0.94 | 0.21 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3239 | 1/1   | 0.94 | 0.21 | 33,33,33,33                 | 0     |
| 54  | MG   | 15    | 104  | 1/1   | 0.94 | 0.15 | 62,62,62,62                 | 0     |
| 54  | MG   | 17    | 101  | 1/1   | 0.94 | 0.49 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 1659 | 1/1   | 0.94 | 0.24 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 1660 | 1/1   | 0.94 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3487 | 1/1   | 0.94 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3176 | 1/1   | 0.94 | 0.21 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3489 | 1/1   | 0.94 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3758 | 1/1   | 0.94 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3494 | 1/1   | 0.94 | 0.21 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3495 | 1/1   | 0.94 | 0.20 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3178 | 1/1   | 0.94 | 0.15 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3288 | 1/1   | 0.94 | 0.16 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3180 | 1/1   | 0.94 | 0.35 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3626 | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1601 | 1/1   | 0.94 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3505 | 1/1   | 0.94 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 1677 | 1/1   | 0.94 | 0.22 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1602 | 1/1   | 0.94 | 0.10 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3764 | 1/1   | 0.94 | 0.20 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3628 | 1/1   | 0.94 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3289 | 1/1   | 0.94 | 0.16 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3634 | 1/1   | 0.94 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3352 | 1/1   | 0.94 | 0.21 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3524 | 1/1   | 0.94 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3777 | 1/1   | 0.94 | 0.10 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3240 | 1/1   | 0.94 | 0.22 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 1692 | 1/1   | 0.94 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3035 | 1/1   | 0.94 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3525 | 1/1   | 0.94 | 0.18 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3527 | 1/1   | 0.94 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 1696 | 1/1   | 0.94 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 1697 | 1/1   | 0.94 | 0.20 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3948 | 1/1   | 0.94 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3529 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1621 | 1/1   | 0.94 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3643 | 1/1   | 0.94 | 0.30 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 1715 | 1/1   | 0.94 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1623 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 1718 | 1/1   | 0.94 | 0.27 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 1719 | 1/1   | 0.94 | 0.16 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3536 | 1/1   | 0.94 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3009 | 1/1   | 0.94 | 0.23 | 34,34,34,34                 | 0     |
| 54  | MG   | 2a    | 1723 | 1/1   | 0.94 | 0.19 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3647 | 1/1   | 0.94 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3295 | 1/1   | 0.94 | 0.17 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3650 | 1/1   | 0.94 | 0.26 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 1730 | 1/1   | 0.94 | 0.22 | 49,49,49,49                 | 0     |
| 54  | MG   | 2a    | 1731 | 1/1   | 0.94 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 1732 | 1/1   | 0.94 | 0.29 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3204 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3531 | 1/1   | 0.94 | 0.37 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 1738 | 1/1   | 0.94 | 0.30 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3790 | 1/1   | 0.94 | 0.17 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1630 | 1/1   | 0.94 | 0.20 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3793 | 1/1   | 0.94 | 0.19 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3210 | 1/1   | 0.94 | 0.13 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3362 | 1/1   | 0.94 | 0.11 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1852 | 1/1   | 0.94 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3557 | 1/1   | 0.94 | 0.13 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3795 | 1/1   | 0.94 | 0.12 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3533 | 1/1   | 0.94 | 0.14 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3247 | 1/1   | 0.94 | 0.22 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3250 | 1/1   | 0.94 | 0.38 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3370 | 1/1   | 0.94 | 0.14 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3568 | 1/1   | 0.94 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3801 | 1/1   | 0.94 | 0.11 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3802 | 1/1   | 0.94 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | 2t    | 3001 | 1/1   | 0.94 | 0.11 | 45,45,45,45                 | 0     |
| 56  | EZP  | 2A    | 3709 | 25/25 | 0.94 | 0.46 | 38,42,50,58                 | 0     |
| 54  | MG   | 1A    | 3023 | 1/1   | 0.94 | 0.12 | 19,19,19,19                 | 0     |
| 54  | MG   | 2A    | 3575 | 1/1   | 0.94 | 0.21 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3223 | 1/1   | 0.94 | 0.89 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3970 | 1/1   | 0.94 | 0.68 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3974 | 1/1   | 0.94 | 0.14 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3583 | 1/1   | 0.94 | 0.14 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3976 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1f    | 3001 | 1/1   | 0.94 | 0.24 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3980 | 1/1   | 0.94 | 0.25 | 48,48,48,48                 | 0     |
| 59  | ZN   | 2n    | 501  | 1/1   | 0.94 | 0.08 | 101,101,101,101             | 0     |
| 54  | MG   | 2A    | 3411 | 1/1   | 0.95 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 1E    | 303  | 1/1   | 0.95 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3557 | 1/1   | 0.95 | 0.13 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3914 | 1/1   | 0.95 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3416 | 1/1   | 0.95 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 1E    | 307  | 1/1   | 0.95 | 0.13 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3681 | 1/1   | 0.95 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3916 | 1/1   | 0.95 | 0.09 | 29,29,29,29                 | 0     |
| 54  | MG   | 1F    | 304  | 1/1   | 0.95 | 0.29 | 24,24,24,24                 | 0     |
| 54  | MG   | 1a    | 1694 | 1/1   | 0.95 | 0.21 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1695 | 1/1   | 0.95 | 0.20 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3466 | 1/1   | 0.95 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3688 | 1/1   | 0.95 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3919 | 1/1   | 0.95 | 0.34 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3389 | 1/1   | 0.95 | 0.15 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3185 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1699 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3923 | 1/1   | 0.95 | 0.23 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3094 | 1/1   | 0.95 | 0.46 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3696 | 1/1   | 0.95 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3926 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3169 | 1/1   | 0.95 | 0.62 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3699 | 1/1   | 0.95 | 0.28 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3275 | 1/1   | 0.95 | 0.21 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3438 | 1/1   | 0.95 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3078 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3440 | 1/1   | 0.95 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3930 | 1/1   | 0.95 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3791 | 1/1   | 0.95 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3708 | 1/1   | 0.95 | 0.15 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3566 | 1/1   | 0.95 | 0.20 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1712 | 1/1   | 0.95 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3237 | 1/1   | 0.95 | 0.24 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3718 | 1/1   | 0.95 | 0.44 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3002 | 1/1   | 0.95 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3568 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3098 | 1/1   | 0.95 | 0.38 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3007 | 1/1   | 0.95 | 0.43 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3333 | 1/1   | 0.95 | 0.13 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3725 | 1/1   | 0.95 | 0.28 | 37,37,37,37                 | 0     |
| 54  | MG   | 1O    | 8002 | 1/1   | 0.95 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1721 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 1P    | 201  | 1/1   | 0.95 | 0.35 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3143 | 1/1   | 0.95 | 0.06 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3682 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 2B    | 3006 | 1/1   | 0.95 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3099 | 1/1   | 0.95 | 0.34 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3401 | 1/1   | 0.95 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 2B    | 3009 | 1/1   | 0.95 | 0.08 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3025 | 1/1   | 0.95 | 0.55 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3025 | 1/1   | 0.95 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3689 | 1/1   | 0.95 | 0.09 | 22,22,22,22                 | 0     |
| 54  | MG   | 1a    | 1736 | 1/1   | 0.95 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3807 | 1/1   | 0.95 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3470 | 1/1   | 0.95 | 0.41 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3945 | 1/1   | 0.95 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3284 | 1/1   | 0.95 | 0.50 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3473 | 1/1   | 0.95 | 0.32 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3947 | 1/1   | 0.95 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3578 | 1/1   | 0.95 | 0.20 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3692 | 1/1   | 0.95 | 0.14 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3812 | 1/1   | 0.95 | 0.44 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3042 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3480 | 1/1   | 0.95 | 0.68 | 37,37,37,37                 | 0     |
| 54  | MG   | 1W    | 3002 | 1/1   | 0.95 | 0.14 | 39,39,39,39                 | 0     |
| 54  | MG   | 2E    | 305  | 1/1   | 0.95 | 0.24 | 52,52,52,52                 | 0     |
| 54  | MG   | 2E    | 306  | 1/1   | 0.95 | 0.51 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3490 | 1/1   | 0.95 | 0.16 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3045 | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3484 | 1/1   | 0.95 | 0.36 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3492 | 1/1   | 0.95 | 0.13 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3065 | 1/1   | 0.95 | 0.40 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3179 | 1/1   | 0.95 | 0.45 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1750 | 1/1   | 0.95 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3497 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3002 | 1/1   | 0.95 | 0.11 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3211 | 1/1   | 0.95 | 0.21 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3498 | 1/1   | 0.95 | 0.17 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3240 | 1/1   | 0.95 | 0.24 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3822 | 1/1   | 0.95 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3152 | 1/1   | 0.95 | 0.23 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3824 | 1/1   | 0.95 | 0.19 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3592 | 1/1   | 0.95 | 0.18 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3022 | 1/1   | 0.95 | 0.23 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3502 | 1/1   | 0.95 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1763 | 1/1   | 0.95 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3061 | 1/1   | 0.95 | 0.27 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3253 | 1/1   | 0.95 | 0.19 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3830 | 1/1   | 0.95 | 0.14 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3511 | 1/1   | 0.95 | 0.22 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3255 | 1/1   | 0.95 | 0.60 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3513 | 1/1   | 0.95 | 0.21 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3709 | 1/1   | 0.95 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3263 | 1/1   | 0.95 | 0.19 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3264 | 1/1   | 0.95 | 0.14 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3973 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3421 | 1/1   | 0.95 | 0.12 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3505 | 1/1   | 0.95 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3271 | 1/1   | 0.95 | 0.11 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1774 | 1/1   | 0.95 | 0.17 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 2A    | 3531 | 1/1   | 0.95 | 0.11 | 54,54,54,54                | 0     |
| 54  | MG   | 2A    | 3074 | 1/1   | 0.95 | 0.41 | 39,39,39,39                | 0     |
| 54  | MG   | 1A    | 3977 | 1/1   | 0.95 | 0.17 | 38,38,38,38                | 0     |
| 54  | MG   | 2A    | 3277 | 1/1   | 0.95 | 0.15 | 38,38,38,38                | 0     |
| 54  | MG   | 2A    | 3535 | 1/1   | 0.95 | 0.07 | 42,42,42,42                | 0     |
| 54  | MG   | 2a    | 1619 | 1/1   | 0.95 | 0.19 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3086 | 1/1   | 0.95 | 0.41 | 26,26,26,26                | 0     |
| 54  | MG   | 1A    | 3110 | 1/1   | 0.95 | 0.24 | 37,37,37,37                | 0     |
| 54  | MG   | 1A    | 3838 | 1/1   | 0.95 | 0.19 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3541 | 1/1   | 0.95 | 0.07 | 47,47,47,47                | 0     |
| 54  | MG   | 2A    | 3543 | 1/1   | 0.95 | 0.27 | 49,49,49,49                | 0     |
| 54  | MG   | 1A    | 3840 | 1/1   | 0.95 | 0.12 | 33,33,33,33                | 0     |
| 54  | MG   | 1a    | 1616 | 1/1   | 0.95 | 0.12 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3546 | 1/1   | 0.95 | 0.26 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 3358 | 1/1   | 0.95 | 0.17 | 21,21,21,21                | 0     |
| 54  | MG   | 2A    | 3288 | 1/1   | 0.95 | 0.12 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3082 | 1/1   | 0.95 | 0.07 | 62,62,62,62                | 0     |
| 54  | MG   | 2a    | 1634 | 1/1   | 0.95 | 0.24 | 55,55,55,55                | 0     |
| 54  | MG   | 2A    | 3550 | 1/1   | 0.95 | 0.16 | 31,31,31,31                | 0     |
| 54  | MG   | 2a    | 1636 | 1/1   | 0.95 | 0.11 | 69,69,69,69                | 0     |
| 54  | MG   | 1A    | 3992 | 1/1   | 0.95 | 0.52 | 28,28,28,28                | 0     |
| 54  | MG   | 2A    | 3292 | 1/1   | 0.95 | 0.23 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3844 | 1/1   | 0.95 | 0.12 | 46,46,46,46                | 0     |
| 54  | MG   | 1a    | 1784 | 1/1   | 0.95 | 0.18 | 59,59,59,59                | 0     |
| 54  | MG   | 2A    | 3295 | 1/1   | 0.95 | 0.17 | 55,55,55,55                | 0     |
| 54  | MG   | 2A    | 3556 | 1/1   | 0.95 | 0.25 | 35,35,35,35                | 0     |
| 54  | MG   | 2a    | 1643 | 1/1   | 0.95 | 0.12 | 55,55,55,55                | 0     |
| 54  | MG   | 1A    | 3299 | 1/1   | 0.95 | 0.17 | 19,19,19,19                | 0     |
| 54  | MG   | 1A    | 3090 | 1/1   | 0.95 | 0.21 | 12,12,12,12                | 0     |
| 54  | MG   | 2a    | 1646 | 1/1   | 0.95 | 0.11 | 63,63,63,63                | 0     |
| 54  | MG   | 1A    | 3517 | 1/1   | 0.95 | 0.18 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3851 | 1/1   | 0.95 | 0.10 | 41,41,41,41                | 0     |
| 54  | MG   | 2A    | 3302 | 1/1   | 0.95 | 0.12 | 25,25,25,25                | 0     |
| 54  | MG   | 1A    | 3518 | 1/1   | 0.95 | 0.57 | 51,51,51,51                | 0     |
| 54  | MG   | 1a    | 1792 | 1/1   | 0.95 | 0.11 | 57,57,57,57                | 0     |
| 54  | MG   | 2A    | 3097 | 1/1   | 0.95 | 0.10 | 67,67,67,67                | 0     |
| 54  | MG   | 1A    | 3219 | 1/1   | 0.95 | 0.27 | 25,25,25,25                | 0     |
| 54  | MG   | 1A    | 3612 | 1/1   | 0.95 | 0.18 | 22,22,22,22                | 0     |
| 54  | MG   | 1A    | 3366 | 1/1   | 0.95 | 0.24 | 16,16,16,16                | 0     |
| 54  | MG   | 2a    | 1657 | 1/1   | 0.95 | 0.11 | 44,44,44,44                | 0     |
| 54  | MG   | 2A    | 3576 | 1/1   | 0.95 | 0.10 | 62,62,62,62                | 0     |
| 54  | MG   | 2A    | 3577 | 1/1   | 0.95 | 0.12 | 68,68,68,68                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3310 | 1/1   | 0.95 | 0.15 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3104 | 1/1   | 0.95 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3135 | 1/1   | 0.95 | 0.15 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3731 | 1/1   | 0.95 | 0.31 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3863 | 1/1   | 0.95 | 0.12 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3368 | 1/1   | 0.95 | 0.19 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3588 | 1/1   | 0.95 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 1668 | 1/1   | 0.95 | 0.19 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3110 | 1/1   | 0.95 | 0.40 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3322 | 1/1   | 0.95 | 0.13 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3523 | 1/1   | 0.95 | 0.19 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3324 | 1/1   | 0.95 | 0.12 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3325 | 1/1   | 0.95 | 0.15 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3013 | 1/1   | 0.95 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3596 | 1/1   | 0.95 | 0.26 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3327 | 1/1   | 0.95 | 0.14 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 4026 | 1/1   | 0.95 | 0.19 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1636 | 1/1   | 0.95 | 0.22 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3439 | 1/1   | 0.95 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1809 | 1/1   | 0.95 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3334 | 1/1   | 0.95 | 0.19 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3603 | 1/1   | 0.95 | 0.22 | 32,32,32,32                 | 0     |
| 54  | MG   | 2a    | 1687 | 1/1   | 0.95 | 0.21 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3604 | 1/1   | 0.95 | 0.13 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3371 | 1/1   | 0.95 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | 2a    | 1690 | 1/1   | 0.95 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1811 | 1/1   | 0.95 | 0.16 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3441 | 1/1   | 0.95 | 0.20 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3745 | 1/1   | 0.95 | 0.27 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1644 | 1/1   | 0.95 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3342 | 1/1   | 0.95 | 0.23 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1647 | 1/1   | 0.95 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1699 | 1/1   | 0.95 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3372 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 1703 | 1/1   | 0.95 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3129 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 1705 | 1/1   | 0.95 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 1706 | 1/1   | 0.95 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3130 | 1/1   | 0.95 | 0.51 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3354 | 1/1   | 0.95 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG   | 2a    | 1710 | 1/1   | 0.95 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 1711 | 1/1   | 0.95 | 0.22 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 1714 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3443 | 1/1   | 0.95 | 0.14 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3623 | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 2a    | 1717 | 1/1   | 0.95 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3444 | 1/1   | 0.95 | 0.14 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3360 | 1/1   | 0.95 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3640 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3628 | 1/1   | 0.95 | 0.07 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 1722 | 1/1   | 0.95 | 0.25 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3262 | 1/1   | 0.95 | 0.15 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3224 | 1/1   | 0.95 | 0.42 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1654 | 1/1   | 0.95 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 1727 | 1/1   | 0.95 | 0.21 | 61,61,61,61                 | 0     |
| 54  | MG   | 1B    | 212  | 1/1   | 0.95 | 0.05 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1656 | 1/1   | 0.95 | 0.20 | 63,63,63,63                 | 0     |
| 54  | MG   | 1B    | 214  | 1/1   | 0.95 | 0.13 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3880 | 1/1   | 0.95 | 0.14 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 1734 | 1/1   | 0.95 | 0.21 | 55,55,55,55                 | 0     |
| 54  | MG   | 1B    | 216  | 1/1   | 0.95 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | 2a    | 1736 | 1/1   | 0.95 | 0.20 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3040 | 1/1   | 0.95 | 0.15 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3052 | 1/1   | 0.95 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 2a    | 1739 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3451 | 1/1   | 0.95 | 0.16 | 15,15,15,15                 | 0     |
| 54  | MG   | 2a    | 1741 | 1/1   | 0.95 | 0.15 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3759 | 1/1   | 0.95 | 0.60 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3381 | 1/1   | 0.95 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 1744 | 1/1   | 0.95 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3380 | 1/1   | 0.95 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | 1B    | 223  | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3382 | 1/1   | 0.95 | 0.14 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3762 | 1/1   | 0.95 | 0.15 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3454 | 1/1   | 0.95 | 0.13 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3655 | 1/1   | 0.95 | 0.16 | 42,42,42,42                 | 0     |
| 54  | MG   | 1B    | 227  | 1/1   | 0.95 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3456 | 1/1   | 0.95 | 0.21 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3387 | 1/1   | 0.95 | 0.23 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3546 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3268 | 1/1   | 0.95 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3391 | 1/1   | 0.95 | 0.16 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3162 | 1/1   | 0.95 | 0.11 | 53,53,53,53                 | 0     |
| 56  | EZP  | 1A    | 3987 | 25/25 | 0.95 | 0.39 | 16,28,47,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3459 | 1/1   | 0.95 | 0.17 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3394 | 1/1   | 0.95 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3770 | 1/1   | 0.95 | 0.18 | 27,27,27,27                 | 0     |
| 57  | MPD  | 18    | 102  | 8/8   | 0.95 | 0.36 | 22,28,35,36                 | 0     |
| 54  | MG   | 1A    | 3385 | 1/1   | 0.95 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3316 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3230 | 1/1   | 0.95 | 0.19 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3168 | 1/1   | 0.95 | 0.12 | 54,54,54,54                 | 0     |
| 58  | ARG  | 1B    | 228  | 12/12 | 0.95 | 0.26 | 26,40,53,54                 | 0     |
| 54  | MG   | 1A    | 3556 | 1/1   | 0.95 | 0.14 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3911 | 1/1   | 0.95 | 0.23 | 46,46,46,46                 | 0     |
| 54  | MG   | 1E    | 302  | 1/1   | 0.95 | 0.77 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3409 | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3445 | 1/1   | 0.96 | 0.37 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3080 | 1/1   | 0.96 | 0.45 | 37,37,37,37                 | 0     |
| 54  | MG   | 1a    | 1713 | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3778 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1G    | 3004 | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3704 | 1/1   | 0.96 | 0.17 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3013 | 1/1   | 0.96 | 0.50 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3451 | 1/1   | 0.96 | 0.16 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1717 | 1/1   | 0.96 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3656 | 1/1   | 0.96 | 0.19 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3465 | 1/1   | 0.96 | 0.19 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3554 | 1/1   | 0.96 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3716 | 1/1   | 0.96 | 0.45 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3555 | 1/1   | 0.96 | 0.18 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3267 | 1/1   | 0.96 | 0.15 | 29,29,29,29                 | 0     |
| 54  | MG   | 1a    | 1725 | 1/1   | 0.96 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3024 | 1/1   | 0.96 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3467 | 1/1   | 0.96 | 0.07 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3464 | 1/1   | 0.96 | 0.16 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3222 | 1/1   | 0.96 | 0.16 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3785 | 1/1   | 0.96 | 0.21 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3468 | 1/1   | 0.96 | 0.16 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3030 | 1/1   | 0.96 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3222 | 1/1   | 0.96 | 0.46 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3325 | 1/1   | 0.96 | 0.27 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1732 | 1/1   | 0.96 | 0.08 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3668 | 1/1   | 0.96 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3232 | 1/1   | 0.96 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3037 | 1/1   | 0.96 | 0.16 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3038 | 1/1   | 0.96 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1735 | 1/1   | 0.96 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3561 | 1/1   | 0.96 | 0.12 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3237 | 1/1   | 0.96 | 0.47 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3326 | 1/1   | 0.96 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3105 | 1/1   | 0.96 | 0.16 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3328 | 1/1   | 0.96 | 0.11 | 13,13,13,13                 | 0     |
| 54  | MG   | 1A    | 3396 | 1/1   | 0.96 | 0.13 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3329 | 1/1   | 0.96 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3012 | 1/1   | 0.96 | 0.20 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3569 | 1/1   | 0.96 | 0.29 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3248 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 1V    | 201  | 1/1   | 0.96 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 2D    | 304  | 1/1   | 0.96 | 0.48 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3490 | 1/1   | 0.96 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 2D    | 306  | 1/1   | 0.96 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3062 | 1/1   | 0.96 | 0.16 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3571 | 1/1   | 0.96 | 0.41 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3228 | 1/1   | 0.96 | 0.22 | 18,18,18,18                 | 0     |
| 54  | MG   | 2A    | 3496 | 1/1   | 0.96 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3497 | 1/1   | 0.96 | 0.14 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3806 | 1/1   | 0.96 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | 2F    | 302  | 1/1   | 0.96 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3254 | 1/1   | 0.96 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3255 | 1/1   | 0.96 | 0.12 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3334 | 1/1   | 0.96 | 0.14 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3260 | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3808 | 1/1   | 0.96 | 0.23 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3276 | 1/1   | 0.96 | 0.25 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3001 | 1/1   | 0.96 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3338 | 1/1   | 0.96 | 0.12 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3405 | 1/1   | 0.96 | 0.14 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3814 | 1/1   | 0.96 | 0.15 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3192 | 1/1   | 0.96 | 0.41 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3494 | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3272 | 1/1   | 0.96 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 13    | 102  | 1/1   | 0.96 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3514 | 1/1   | 0.96 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3518 | 1/1   | 0.96 | 0.11 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3067 | 1/1   | 0.96 | 0.45 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1762 | 1/1   | 0.96 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3580 | 1/1   | 0.96 | 0.15 | 22,22,22,22                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3523 | 1/1   | 0.96 | 0.23 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1765 | 1/1   | 0.96 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | 15    | 103  | 1/1   | 0.96 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3526 | 1/1   | 0.96 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3282 | 1/1   | 0.96 | 0.17 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3409 | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3695 | 1/1   | 0.96 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1769 | 1/1   | 0.96 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3286 | 1/1   | 0.96 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1770 | 1/1   | 0.96 | 0.19 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 1610 | 1/1   | 0.96 | 0.23 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3340 | 1/1   | 0.96 | 0.12 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3289 | 1/1   | 0.96 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 18    | 101  | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3232 | 1/1   | 0.96 | 0.48 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3539 | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3698 | 1/1   | 0.96 | 0.20 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3699 | 1/1   | 0.96 | 0.13 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3542 | 1/1   | 0.96 | 0.19 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3972 | 1/1   | 0.96 | 0.36 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3193 | 1/1   | 0.96 | 0.22 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3588 | 1/1   | 0.96 | 0.16 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3085 | 1/1   | 0.96 | 0.16 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3053 | 1/1   | 0.96 | 0.22 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3300 | 1/1   | 0.96 | 0.14 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3827 | 1/1   | 0.96 | 0.16 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3089 | 1/1   | 0.96 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1610 | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 1628 | 1/1   | 0.96 | 0.11 | 31,31,31,31                 | 0     |
| 54  | MG   | 2a    | 1629 | 1/1   | 0.96 | 0.21 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1611 | 1/1   | 0.96 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3088 | 1/1   | 0.96 | 0.25 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3168 | 1/1   | 0.96 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 1633 | 1/1   | 0.96 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1614 | 1/1   | 0.96 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3068 | 1/1   | 0.96 | 0.15 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1787 | 1/1   | 0.96 | 0.25 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3312 | 1/1   | 0.96 | 0.20 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3561 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3099 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3200 | 1/1   | 0.96 | 0.34 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3564 | 1/1   | 0.96 | 0.12 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3565 | 1/1   | 0.96 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3424 | 1/1   | 0.96 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1790 | 1/1   | 0.96 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3319 | 1/1   | 0.96 | 0.16 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3990 | 1/1   | 0.96 | 0.23 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3991 | 1/1   | 0.96 | 0.58 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3069 | 1/1   | 0.96 | 0.18 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3993 | 1/1   | 0.96 | 0.26 | 26,26,26,26                 | 0     |
| 54  | MG   | 1a    | 1795 | 1/1   | 0.96 | 0.28 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3032 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 1652 | 1/1   | 0.96 | 0.19 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3204 | 1/1   | 0.96 | 0.52 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3356 | 1/1   | 0.96 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3839 | 1/1   | 0.96 | 0.25 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3429 | 1/1   | 0.96 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3244 | 1/1   | 0.96 | 0.38 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3331 | 1/1   | 0.96 | 0.16 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3716 | 1/1   | 0.96 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3846 | 1/1   | 0.96 | 0.13 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3121 | 1/1   | 0.96 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3046 | 1/1   | 0.96 | 0.36 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3337 | 1/1   | 0.96 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3206 | 1/1   | 0.96 | 0.23 | 18,18,18,18                 | 0     |
| 54  | MG   | 2a    | 1665 | 1/1   | 0.96 | 0.33 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3719 | 1/1   | 0.96 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3207 | 1/1   | 0.96 | 0.43 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3438 | 1/1   | 0.96 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 4020 | 1/1   | 0.96 | 0.54 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3345 | 1/1   | 0.96 | 0.29 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3347 | 1/1   | 0.96 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 4021 | 1/1   | 0.96 | 0.52 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3722 | 1/1   | 0.96 | 0.22 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3723 | 1/1   | 0.96 | 0.13 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3352 | 1/1   | 0.96 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3353 | 1/1   | 0.96 | 0.21 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 1679 | 1/1   | 0.96 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 4024 | 1/1   | 0.96 | 0.50 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3072 | 1/1   | 0.96 | 0.49 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3356 | 1/1   | 0.96 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3074 | 1/1   | 0.96 | 0.44 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3359 | 1/1   | 0.96 | 0.14 | 52,52,52,52                 | 0     |
| 54  | MG   | 1B    | 201  | 1/1   | 0.96 | 0.53 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3007 | 1/1   | 0.96 | 0.13 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3369 | 1/1   | 0.96 | 0.17 | 16,16,16,16                 | 0     |
| 54  | MG   | 1a    | 1823 | 1/1   | 0.96 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3729 | 1/1   | 0.96 | 0.18 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3620 | 1/1   | 0.96 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3617 | 1/1   | 0.96 | 0.15 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3622 | 1/1   | 0.96 | 0.17 | 18,18,18,18                 | 0     |
| 54  | MG   | 1a    | 1826 | 1/1   | 0.96 | 0.21 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3150 | 1/1   | 0.96 | 0.69 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3028 | 1/1   | 0.96 | 0.13 | 30,30,30,30                 | 0     |
| 54  | MG   | 2a    | 1698 | 1/1   | 0.96 | 0.19 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3304 | 1/1   | 0.96 | 0.17 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3734 | 1/1   | 0.96 | 0.26 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3622 | 1/1   | 0.96 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3623 | 1/1   | 0.96 | 0.13 | 32,32,32,32                 | 0     |
| 54  | MG   | 1B    | 213  | 1/1   | 0.96 | 0.18 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3155 | 1/1   | 0.96 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1661 | 1/1   | 0.96 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3738 | 1/1   | 0.96 | 0.14 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3158 | 1/1   | 0.96 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3624 | 1/1   | 0.96 | 0.32 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 1712 | 1/1   | 0.96 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3741 | 1/1   | 0.96 | 0.15 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3641 | 1/1   | 0.96 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3742 | 1/1   | 0.96 | 0.14 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3743 | 1/1   | 0.96 | 0.24 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3645 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3049 | 1/1   | 0.96 | 0.38 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3374 | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3746 | 1/1   | 0.96 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3629 | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1847 | 1/1   | 0.96 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3630 | 1/1   | 0.96 | 0.24 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1849 | 1/1   | 0.96 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3885 | 1/1   | 0.96 | 0.20 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 1728 | 1/1   | 0.96 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3886 | 1/1   | 0.96 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3750 | 1/1   | 0.96 | 0.16 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3400 | 1/1   | 0.96 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3889 | 1/1   | 0.96 | 0.19 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3631 | 1/1   | 0.96 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3404 | 1/1   | 0.96 | 0.15 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3892 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3307 | 1/1   | 0.96 | 0.17 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3450 | 1/1   | 0.96 | 0.22 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3754 | 1/1   | 0.96 | 0.40 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3410 | 1/1   | 0.96 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3377 | 1/1   | 0.96 | 0.20 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3181 | 1/1   | 0.96 | 0.18 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3636 | 1/1   | 0.96 | 0.22 | 17,17,17,17                 | 0     |
| 54  | MG   | 1D    | 312  | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3153 | 1/1   | 0.96 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3639 | 1/1   | 0.96 | 0.21 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3418 | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3215 | 1/1   | 0.96 | 0.31 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3187 | 1/1   | 0.96 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 1750 | 1/1   | 0.96 | 0.08 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3216 | 1/1   | 0.96 | 0.55 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3455 | 1/1   | 0.96 | 0.16 | 10,10,10,10                 | 0     |
| 54  | MG   | 2A    | 3678 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3907 | 1/1   | 0.96 | 0.14 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3029 | 1/1   | 0.96 | 0.14 | 12,12,12,12                 | 0     |
| 54  | MG   | 1F    | 301  | 1/1   | 0.96 | 0.75 | 41,41,41,41                 | 0     |
| 54  | MG   | 1i    | 3001 | 1/1   | 0.96 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3909 | 1/1   | 0.96 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1F    | 303  | 1/1   | 0.96 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3644 | 1/1   | 0.96 | 0.08 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3686 | 1/1   | 0.96 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3433 | 1/1   | 0.96 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3129 | 1/1   | 0.96 | 0.43 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3689 | 1/1   | 0.96 | 0.06 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3318 | 1/1   | 0.96 | 0.17 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3547 | 1/1   | 0.96 | 0.15 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3386 | 1/1   | 0.96 | 0.12 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3186 | 1/1   | 0.96 | 0.47 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3462 | 1/1   | 0.96 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1708 | 1/1   | 0.96 | 0.24 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3922 | 1/1   | 0.96 | 0.27 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3775 | 1/1   | 0.96 | 0.26 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3145 | 1/1   | 0.97 | 0.50 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1745 | 1/1   | 0.97 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3146 | 1/1   | 0.97 | 0.83 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3008 | 1/1   | 0.97 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3027 | 1/1   | 0.97 | 0.26 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 2E    | 301  | 1/1   | 0.97 | 0.12 | 43,43,43,43                | 0     |
| 54  | MG   | 2A    | 3351 | 1/1   | 0.97 | 0.17 | 25,25,25,25                | 0     |
| 54  | MG   | 2E    | 303  | 1/1   | 0.97 | 0.09 | 44,44,44,44                | 0     |
| 54  | MG   | 2A    | 3011 | 1/1   | 0.97 | 0.13 | 21,21,21,21                | 0     |
| 54  | MG   | 1A    | 3918 | 1/1   | 0.97 | 0.16 | 38,38,38,38                | 0     |
| 54  | MG   | 1a    | 1615 | 1/1   | 0.97 | 0.17 | 59,59,59,59                | 0     |
| 54  | MG   | 1A    | 3020 | 1/1   | 0.97 | 0.25 | 33,33,33,33                | 0     |
| 54  | MG   | 2A    | 3015 | 1/1   | 0.97 | 0.42 | 43,43,43,43                | 0     |
| 54  | MG   | 1A    | 3653 | 1/1   | 0.97 | 0.45 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 3245 | 1/1   | 0.97 | 0.11 | 27,27,27,27                | 0     |
| 54  | MG   | 2A    | 3018 | 1/1   | 0.97 | 0.13 | 40,40,40,40                | 0     |
| 54  | MG   | 1A    | 3507 | 1/1   | 0.97 | 0.10 | 29,29,29,29                | 0     |
| 54  | MG   | 2A    | 3020 | 1/1   | 0.97 | 0.31 | 57,57,57,57                | 0     |
| 54  | MG   | 2O    | 201  | 1/1   | 0.97 | 0.12 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3246 | 1/1   | 0.97 | 0.14 | 58,58,58,58                | 0     |
| 54  | MG   | 2A    | 3364 | 1/1   | 0.97 | 0.26 | 58,58,58,58                | 0     |
| 54  | MG   | 2A    | 3366 | 1/1   | 0.97 | 0.14 | 31,31,31,31                | 0     |
| 54  | MG   | 1A    | 3925 | 1/1   | 0.97 | 0.14 | 49,49,49,49                | 0     |
| 54  | MG   | 1A    | 3658 | 1/1   | 0.97 | 0.10 | 24,24,24,24                | 0     |
| 54  | MG   | 1A    | 3509 | 1/1   | 0.97 | 0.14 | 41,41,41,41                | 0     |
| 54  | MG   | 2T    | 3003 | 1/1   | 0.97 | 0.16 | 61,61,61,61                | 0     |
| 54  | MG   | 2T    | 3004 | 1/1   | 0.97 | 0.10 | 44,44,44,44                | 0     |
| 54  | MG   | 1A    | 3447 | 1/1   | 0.97 | 0.15 | 34,34,34,34                | 0     |
| 54  | MG   | 1A    | 3149 | 1/1   | 0.97 | 0.25 | 21,21,21,21                | 0     |
| 54  | MG   | 1A    | 3248 | 1/1   | 0.97 | 0.14 | 31,31,31,31                | 0     |
| 54  | MG   | 1A    | 3931 | 1/1   | 0.97 | 0.21 | 34,34,34,34                | 0     |
| 54  | MG   | 1A    | 3515 | 1/1   | 0.97 | 0.29 | 30,30,30,30                | 0     |
| 54  | MG   | 1A    | 3249 | 1/1   | 0.97 | 0.41 | 34,34,34,34                | 0     |
| 54  | MG   | 2A    | 3571 | 1/1   | 0.97 | 0.20 | 42,42,42,42                | 0     |
| 54  | MG   | 2A    | 3376 | 1/1   | 0.97 | 0.10 | 47,47,47,47                | 0     |
| 54  | MG   | 2A    | 3574 | 1/1   | 0.97 | 0.15 | 52,52,52,52                | 0     |
| 54  | MG   | 2A    | 3033 | 1/1   | 0.97 | 0.17 | 46,46,46,46                | 0     |
| 54  | MG   | 1A    | 3033 | 1/1   | 0.97 | 0.21 | 34,34,34,34                | 0     |
| 54  | MG   | 2A    | 3035 | 1/1   | 0.97 | 0.13 | 29,29,29,29                | 0     |
| 54  | MG   | 2A    | 3578 | 1/1   | 0.97 | 0.16 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3294 | 1/1   | 0.97 | 0.10 | 46,46,46,46                | 0     |
| 54  | MG   | 2A    | 3580 | 1/1   | 0.97 | 0.17 | 36,36,36,36                | 0     |
| 54  | MG   | 1a    | 1632 | 1/1   | 0.97 | 0.13 | 35,35,35,35                | 0     |
| 54  | MG   | 1A    | 3586 | 1/1   | 0.97 | 0.10 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3587 | 1/1   | 0.97 | 0.15 | 26,26,26,26                | 0     |
| 54  | MG   | 2A    | 3584 | 1/1   | 0.97 | 0.13 | 46,46,46,46                | 0     |
| 54  | MG   | 1A    | 3126 | 1/1   | 0.97 | 0.48 | 33,33,33,33                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3087 | 1/1   | 0.97 | 0.53 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3041 | 1/1   | 0.97 | 0.12 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3254 | 1/1   | 0.97 | 0.36 | 30,30,30,30                 | 0     |
| 54  | MG   | 1D    | 308  | 1/1   | 0.97 | 0.27 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3390 | 1/1   | 0.97 | 0.13 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3592 | 1/1   | 0.97 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3348 | 1/1   | 0.97 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1642 | 1/1   | 0.97 | 0.20 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3209 | 1/1   | 0.97 | 0.65 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1643 | 1/1   | 0.97 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3395 | 1/1   | 0.97 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3676 | 1/1   | 0.97 | 0.17 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1645 | 1/1   | 0.97 | 0.19 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1646 | 1/1   | 0.97 | 0.23 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3458 | 1/1   | 0.97 | 0.19 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3596 | 1/1   | 0.97 | 0.40 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3154 | 1/1   | 0.97 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3350 | 1/1   | 0.97 | 0.17 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3849 | 1/1   | 0.97 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3529 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3057 | 1/1   | 0.97 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3221 | 1/1   | 0.97 | 0.40 | 57,57,57,57                 | 0     |
| 54  | MG   | 1E    | 304  | 1/1   | 0.97 | 0.17 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3600 | 1/1   | 0.97 | 0.21 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3852 | 1/1   | 0.97 | 0.32 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3685 | 1/1   | 0.97 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3062 | 1/1   | 0.97 | 0.43 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3615 | 1/1   | 0.97 | 0.14 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3616 | 1/1   | 0.97 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3227 | 1/1   | 0.97 | 0.66 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3228 | 1/1   | 0.97 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3855 | 1/1   | 0.97 | 0.18 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3856 | 1/1   | 0.97 | 0.19 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3107 | 1/1   | 0.97 | 0.26 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3157 | 1/1   | 0.97 | 0.13 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3069 | 1/1   | 0.97 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 1F    | 305  | 1/1   | 0.97 | 0.49 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1798 | 1/1   | 0.97 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3427 | 1/1   | 0.97 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3130 | 1/1   | 0.97 | 0.61 | 25,25,25,25                 | 0     |
| 54  | MG   | 1a    | 1663 | 1/1   | 0.97 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3959 | 1/1   | 0.97 | 0.48 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1F    | 308  | 1/1   | 0.97 | 0.39 | 29,29,29,29                | 0     |
| 54  | MG   | 1a    | 1804 | 1/1   | 0.97 | 0.18 | 59,59,59,59                | 0     |
| 54  | MG   | 2A    | 3634 | 1/1   | 0.97 | 0.15 | 42,42,42,42                | 0     |
| 54  | MG   | 1A    | 3073 | 1/1   | 0.97 | 0.40 | 30,30,30,30                | 0     |
| 54  | MG   | 1A    | 3406 | 1/1   | 0.97 | 0.15 | 52,52,52,52                | 0     |
| 54  | MG   | 2A    | 3638 | 1/1   | 0.97 | 0.09 | 32,32,32,32                | 0     |
| 54  | MG   | 1A    | 3607 | 1/1   | 0.97 | 0.14 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3771 | 1/1   | 0.97 | 0.22 | 27,27,27,27                | 0     |
| 54  | MG   | 2A    | 3437 | 1/1   | 0.97 | 0.08 | 58,58,58,58                | 0     |
| 54  | MG   | 1A    | 3772 | 1/1   | 0.97 | 0.44 | 24,24,24,24                | 0     |
| 54  | MG   | 1a    | 1672 | 1/1   | 0.97 | 0.27 | 51,51,51,51                | 0     |
| 54  | MG   | 1A    | 3109 | 1/1   | 0.97 | 0.57 | 31,31,31,31                | 0     |
| 54  | MG   | 1A    | 3357 | 1/1   | 0.97 | 0.13 | 20,20,20,20                | 0     |
| 54  | MG   | 1A    | 3410 | 1/1   | 0.97 | 0.17 | 18,18,18,18                | 0     |
| 54  | MG   | 2A    | 3086 | 1/1   | 0.97 | 0.13 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3541 | 1/1   | 0.97 | 0.17 | 19,19,19,19                | 0     |
| 54  | MG   | 2a    | 1671 | 1/1   | 0.97 | 0.25 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3042 | 1/1   | 0.97 | 0.23 | 8,8,8,8                    | 0     |
| 54  | MG   | 2A    | 3256 | 1/1   | 0.97 | 0.17 | 51,51,51,51                | 0     |
| 54  | MG   | 2a    | 1674 | 1/1   | 0.97 | 0.16 | 43,43,43,43                | 0     |
| 54  | MG   | 1A    | 3472 | 1/1   | 0.97 | 0.14 | 20,20,20,20                | 0     |
| 54  | MG   | 2A    | 3259 | 1/1   | 0.97 | 0.10 | 32,32,32,32                | 0     |
| 54  | MG   | 1A    | 3360 | 1/1   | 0.97 | 0.16 | 18,18,18,18                | 0     |
| 54  | MG   | 1A    | 3975 | 1/1   | 0.97 | 0.09 | 39,39,39,39                | 0     |
| 54  | MG   | 1A    | 3414 | 1/1   | 0.97 | 0.14 | 49,49,49,49                | 0     |
| 54  | MG   | 1a    | 1682 | 1/1   | 0.97 | 0.10 | 59,59,59,59                | 0     |
| 54  | MG   | 2A    | 3455 | 1/1   | 0.97 | 0.08 | 48,48,48,48                | 0     |
| 54  | MG   | 1a    | 1683 | 1/1   | 0.97 | 0.13 | 59,59,59,59                | 0     |
| 54  | MG   | 1A    | 3308 | 1/1   | 0.97 | 0.20 | 34,34,34,34                | 0     |
| 54  | MG   | 2A    | 3267 | 1/1   | 0.97 | 0.14 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3978 | 1/1   | 0.97 | 0.34 | 26,26,26,26                | 0     |
| 54  | MG   | 2a    | 1686 | 1/1   | 0.97 | 0.09 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3979 | 1/1   | 0.97 | 0.28 | 47,47,47,47                | 0     |
| 54  | MG   | 2A    | 3270 | 1/1   | 0.97 | 0.07 | 37,37,37,37                | 0     |
| 54  | MG   | 2A    | 3100 | 1/1   | 0.97 | 0.16 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3478 | 1/1   | 0.97 | 0.17 | 16,16,16,16                | 0     |
| 54  | MG   | 2a    | 1691 | 1/1   | 0.97 | 0.17 | 56,56,56,56                | 0     |
| 54  | MG   | 2A    | 3102 | 1/1   | 0.97 | 0.11 | 42,42,42,42                | 0     |
| 54  | MG   | 1a    | 1827 | 1/1   | 0.97 | 0.11 | 33,33,33,33                | 0     |
| 54  | MG   | 1A    | 3134 | 1/1   | 0.97 | 0.15 | 22,22,22,22                | 0     |
| 54  | MG   | 1a    | 1829 | 1/1   | 0.97 | 0.18 | 42,42,42,42                | 0     |
| 54  | MG   | 2A    | 3279 | 1/1   | 0.97 | 0.12 | 63,63,63,63                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1Q    | 201  | 1/1   | 0.97 | 0.12 | 38,38,38,38                | 0     |
| 54  | MG   | 1Q    | 202  | 1/1   | 0.97 | 0.14 | 29,29,29,29                | 0     |
| 54  | MG   | 1Q    | 204  | 1/1   | 0.97 | 0.17 | 31,31,31,31                | 0     |
| 54  | MG   | 1A    | 3227 | 1/1   | 0.97 | 0.35 | 25,25,25,25                | 0     |
| 54  | MG   | 2a    | 1701 | 1/1   | 0.97 | 0.26 | 42,42,42,42                | 0     |
| 54  | MG   | 2a    | 1702 | 1/1   | 0.97 | 0.13 | 73,73,73,73                | 0     |
| 54  | MG   | 2A    | 3474 | 1/1   | 0.97 | 0.13 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3482 | 1/1   | 0.97 | 0.18 | 17,17,17,17                | 0     |
| 54  | MG   | 1A    | 3984 | 1/1   | 0.97 | 0.12 | 37,37,37,37                | 0     |
| 54  | MG   | 1A    | 3364 | 1/1   | 0.97 | 0.18 | 13,13,13,13                | 0     |
| 54  | MG   | 1A    | 3989 | 1/1   | 0.97 | 0.32 | 50,50,50,50                | 0     |
| 54  | MG   | 2a    | 1708 | 1/1   | 0.97 | 0.27 | 52,52,52,52                | 0     |
| 54  | MG   | 1a    | 1838 | 1/1   | 0.97 | 0.11 | 55,55,55,55                | 0     |
| 54  | MG   | 1A    | 3312 | 1/1   | 0.97 | 0.18 | 17,17,17,17                | 0     |
| 54  | MG   | 1A    | 3792 | 1/1   | 0.97 | 0.14 | 12,12,12,12                | 0     |
| 54  | MG   | 1A    | 3111 | 1/1   | 0.97 | 0.45 | 31,31,31,31                | 0     |
| 54  | MG   | 2a    | 1713 | 1/1   | 0.97 | 0.43 | 55,55,55,55                | 0     |
| 54  | MG   | 1A    | 3314 | 1/1   | 0.97 | 0.14 | 46,46,46,46                | 0     |
| 54  | MG   | 1A    | 3710 | 1/1   | 0.97 | 0.16 | 38,38,38,38                | 0     |
| 54  | MG   | 1A    | 3997 | 1/1   | 0.97 | 0.25 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3888 | 1/1   | 0.97 | 0.12 | 18,18,18,18                | 0     |
| 54  | MG   | 2A    | 3125 | 1/1   | 0.97 | 0.20 | 38,38,38,38                | 0     |
| 54  | MG   | 1A    | 3796 | 1/1   | 0.97 | 0.19 | 45,45,45,45                | 0     |
| 54  | MG   | 1A    | 4001 | 1/1   | 0.97 | 0.20 | 37,37,37,37                | 0     |
| 54  | MG   | 2A    | 3299 | 1/1   | 0.97 | 0.16 | 28,28,28,28                | 0     |
| 54  | MG   | 2A    | 3128 | 1/1   | 0.97 | 0.53 | 45,45,45,45                | 0     |
| 54  | MG   | 1X    | 102  | 1/1   | 0.97 | 0.16 | 31,31,31,31                | 0     |
| 54  | MG   | 2a    | 1724 | 1/1   | 0.97 | 0.20 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 4002 | 1/1   | 0.97 | 0.63 | 29,29,29,29                | 0     |
| 54  | MG   | 1a    | 1710 | 1/1   | 0.97 | 0.12 | 63,63,63,63                | 0     |
| 54  | MG   | 1A    | 3018 | 1/1   | 0.97 | 0.41 | 24,24,24,24                | 0     |
| 54  | MG   | 2A    | 3499 | 1/1   | 0.97 | 0.21 | 30,30,30,30                | 0     |
| 54  | MG   | 2A    | 3701 | 1/1   | 0.97 | 0.17 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3113 | 1/1   | 0.97 | 0.15 | 18,18,18,18                | 0     |
| 54  | MG   | 1A    | 3893 | 1/1   | 0.97 | 0.11 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3307 | 1/1   | 0.97 | 0.19 | 51,51,51,51                | 0     |
| 54  | MG   | 2a    | 1733 | 1/1   | 0.97 | 0.32 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3231 | 1/1   | 0.97 | 0.52 | 34,34,34,34                | 0     |
| 54  | MG   | 1A    | 3897 | 1/1   | 0.97 | 0.17 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3491 | 1/1   | 0.97 | 0.07 | 36,36,36,36                | 0     |
| 54  | MG   | 11    | 101  | 1/1   | 0.97 | 0.23 | 44,44,44,44                | 0     |
| 54  | MG   | 2A    | 3313 | 1/1   | 0.97 | 0.12 | 33,33,33,33                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 2A    | 3714 | 1/1   | 0.97 | 0.88 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3141 | 1/1   | 0.97 | 0.37 | 39,39,39,39                | 0     |
| 54  | MG   | 1A    | 4011 | 1/1   | 0.97 | 0.33 | 29,29,29,29                | 0     |
| 54  | MG   | 1A    | 3715 | 1/1   | 0.97 | 0.11 | 19,19,19,19                | 0     |
| 54  | MG   | 1A    | 3063 | 1/1   | 0.97 | 0.24 | 32,32,32,32                | 0     |
| 54  | MG   | 1a    | 1722 | 1/1   | 0.97 | 0.15 | 56,56,56,56                | 0     |
| 54  | MG   | 1e    | 3001 | 1/1   | 0.97 | 0.36 | 56,56,56,56                | 0     |
| 54  | MG   | 14    | 502  | 1/1   | 0.97 | 0.06 | 72,72,72,72                | 0     |
| 54  | MG   | 2A    | 3722 | 1/1   | 0.97 | 0.30 | 48,48,48,48                | 0     |
| 54  | MG   | 2A    | 3516 | 1/1   | 0.97 | 0.20 | 19,19,19,19                | 0     |
| 54  | MG   | 2A    | 3517 | 1/1   | 0.97 | 0.20 | 46,46,46,46                | 0     |
| 54  | MG   | 1A    | 3044 | 1/1   | 0.97 | 0.15 | 23,23,23,23                | 0     |
| 54  | MG   | 2A    | 3150 | 1/1   | 0.97 | 0.15 | 62,62,62,62                | 0     |
| 54  | MG   | 1A    | 3234 | 1/1   | 0.97 | 0.49 | 24,24,24,24                | 0     |
| 54  | MG   | 1A    | 4019 | 1/1   | 0.97 | 0.21 | 29,29,29,29                | 0     |
| 54  | MG   | 2A    | 3522 | 1/1   | 0.97 | 0.15 | 47,47,47,47                | 0     |
| 54  | MG   | 1a    | 1728 | 1/1   | 0.97 | 0.10 | 51,51,51,51                | 0     |
| 54  | MG   | 1A    | 3638 | 1/1   | 0.97 | 0.09 | 38,38,38,38                | 0     |
| 54  | MG   | 1A    | 3375 | 1/1   | 0.97 | 0.15 | 16,16,16,16                | 0     |
| 54  | MG   | 1A    | 3564 | 1/1   | 0.97 | 0.11 | 39,39,39,39                | 0     |
| 54  | MG   | 1A    | 3066 | 1/1   | 0.97 | 0.50 | 30,30,30,30                | 0     |
| 54  | MG   | 1a    | 1733 | 1/1   | 0.97 | 0.12 | 55,55,55,55                | 0     |
| 54  | MG   | 1A    | 3097 | 1/1   | 0.97 | 0.58 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3045 | 1/1   | 0.97 | 0.22 | 35,35,35,35                | 0     |
| 54  | MG   | 1A    | 3015 | 1/1   | 0.97 | 0.55 | 29,29,29,29                | 0     |
| 54  | MG   | 1a    | 1603 | 1/1   | 0.97 | 0.15 | 45,45,45,45                | 0     |
| 54  | MG   | 1A    | 3910 | 1/1   | 0.97 | 0.12 | 59,59,59,59                | 0     |
| 54  | MG   | 2B    | 3016 | 1/1   | 0.97 | 0.14 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3813 | 1/1   | 0.97 | 0.13 | 56,56,56,56                | 0     |
| 54  | MG   | 1A    | 3912 | 1/1   | 0.97 | 0.21 | 43,43,43,43                | 0     |
| 54  | MG   | 2A    | 3537 | 1/1   | 0.97 | 0.15 | 42,42,42,42                | 0     |
| 54  | MG   | 1A    | 3176 | 1/1   | 0.97 | 0.17 | 49,49,49,49                | 0     |
| 54  | MG   | 1a    | 1609 | 1/1   | 0.97 | 0.34 | 51,51,51,51                | 0     |
| 59  | ZN   | 29    | 501  | 1/1   | 0.97 | 0.12 | 62,62,62,62                | 0     |
| 54  | MG   | 1B    | 205  | 1/1   | 0.97 | 0.11 | 40,40,40,40                | 0     |
| 54  | MG   | 1A    | 3999 | 1/1   | 0.98 | 0.53 | 32,32,32,32                | 0     |
| 54  | MG   | 2A    | 3316 | 1/1   | 0.98 | 0.18 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 3433 | 1/1   | 0.98 | 0.12 | 32,32,32,32                | 0     |
| 54  | MG   | 1a    | 1801 | 1/1   | 0.98 | 0.15 | 43,43,43,43                | 0     |
| 54  | MG   | 1A    | 3896 | 1/1   | 0.98 | 0.12 | 22,22,22,22                | 0     |
| 54  | MG   | 1A    | 3273 | 1/1   | 0.98 | 0.11 | 30,30,30,30                | 0     |
| 54  | MG   | 1A    | 3435 | 1/1   | 0.98 | 0.22 | 37,37,37,37                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3633 | 1/1   | 0.98 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 4006 | 1/1   | 0.98 | 0.23 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3384 | 1/1   | 0.98 | 0.15 | 14,14,14,14                 | 0     |
| 54  | MG   | 2A    | 3637 | 1/1   | 0.98 | 0.15 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3803 | 1/1   | 0.98 | 0.48 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3306 | 1/1   | 0.98 | 0.13 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3495 | 1/1   | 0.98 | 0.14 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3344 | 1/1   | 0.98 | 0.12 | 21,21,21,21                 | 0     |
| 54  | MG   | 1a    | 1693 | 1/1   | 0.98 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3643 | 1/1   | 0.98 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3345 | 1/1   | 0.98 | 0.22 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3202 | 1/1   | 0.98 | 0.66 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3485 | 1/1   | 0.98 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1815 | 1/1   | 0.98 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3333 | 1/1   | 0.98 | 0.09 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 4015 | 1/1   | 0.98 | 0.38 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3225 | 1/1   | 0.98 | 0.30 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3164 | 1/1   | 0.98 | 0.44 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3653 | 1/1   | 0.98 | 0.28 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3491 | 1/1   | 0.98 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3492 | 1/1   | 0.98 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 4018 | 1/1   | 0.98 | 0.23 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3064 | 1/1   | 0.98 | 0.23 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3277 | 1/1   | 0.98 | 0.35 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3340 | 1/1   | 0.98 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3066 | 1/1   | 0.98 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3165 | 1/1   | 0.98 | 0.35 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3725 | 1/1   | 0.98 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3344 | 1/1   | 0.98 | 0.17 | 37,37,37,37                 | 0     |
| 54  | MG   | 13    | 101  | 1/1   | 0.98 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3393 | 1/1   | 0.98 | 0.17 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3351 | 1/1   | 0.98 | 0.14 | 18,18,18,18                 | 0     |
| 54  | MG   | 1a    | 1706 | 1/1   | 0.98 | 0.17 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3037 | 1/1   | 0.98 | 0.16 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 4025 | 1/1   | 0.98 | 0.37 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3648 | 1/1   | 0.98 | 0.21 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3185 | 1/1   | 0.98 | 0.31 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3024 | 1/1   | 0.98 | 0.33 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3103 | 1/1   | 0.98 | 0.47 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3920 | 1/1   | 0.98 | 0.15 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3357 | 1/1   | 0.98 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3652 | 1/1   | 0.98 | 0.29 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3317 | 1/1   | 0.98 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3515 | 1/1   | 0.98 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3510 | 1/1   | 0.98 | 0.15 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3736 | 1/1   | 0.98 | 0.16 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3114 | 1/1   | 0.98 | 0.15 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3319 | 1/1   | 0.98 | 0.14 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3359 | 1/1   | 0.98 | 0.14 | 15,15,15,15                 | 0     |
| 54  | MG   | 1a    | 1607 | 1/1   | 0.98 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3171 | 1/1   | 0.98 | 0.23 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1724 | 1/1   | 0.98 | 0.18 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3090 | 1/1   | 0.98 | 0.14 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3516 | 1/1   | 0.98 | 0.14 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3285 | 1/1   | 0.98 | 0.29 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3115 | 1/1   | 0.98 | 0.17 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3155 | 1/1   | 0.98 | 0.19 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3834 | 1/1   | 0.98 | 0.14 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3530 | 1/1   | 0.98 | 0.13 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3585 | 1/1   | 0.98 | 0.11 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1850 | 1/1   | 0.98 | 0.07 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3747 | 1/1   | 0.98 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3378 | 1/1   | 0.98 | 0.10 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3407 | 1/1   | 0.98 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3104 | 1/1   | 0.98 | 0.38 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3365 | 1/1   | 0.98 | 0.15 | 13,13,13,13                 | 0     |
| 54  | MG   | 1A    | 3290 | 1/1   | 0.98 | 0.16 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3064 | 1/1   | 0.98 | 0.40 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3842 | 1/1   | 0.98 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3671 | 1/1   | 0.98 | 0.10 | 15,15,15,15                 | 0     |
| 54  | MG   | 2A    | 3107 | 1/1   | 0.98 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3845 | 1/1   | 0.98 | 0.17 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3241 | 1/1   | 0.98 | 0.20 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3525 | 1/1   | 0.98 | 0.17 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3464 | 1/1   | 0.98 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3713 | 1/1   | 0.98 | 0.82 | 40,40,40,40                 | 0     |
| 54  | MG   | 1D    | 301  | 1/1   | 0.98 | 0.30 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3593 | 1/1   | 0.98 | 0.16 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3412 | 1/1   | 0.98 | 0.16 | 45,45,45,45                 | 0     |
| 54  | MG   | 1D    | 305  | 1/1   | 0.98 | 0.26 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3595 | 1/1   | 0.98 | 0.20 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3396 | 1/1   | 0.98 | 0.21 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3096 | 1/1   | 0.98 | 0.33 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3195 | 1/1   | 0.98 | 0.33 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3119 | 1/1   | 0.98 | 0.09 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3853 | 1/1   | 0.98 | 0.14 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3089 | 1/1   | 0.98 | 0.29 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3416 | 1/1   | 0.98 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3559 | 1/1   | 0.98 | 0.19 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3763 | 1/1   | 0.98 | 0.24 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3470 | 1/1   | 0.98 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3956 | 1/1   | 0.98 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3407 | 1/1   | 0.98 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3331 | 1/1   | 0.98 | 0.10 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3684 | 1/1   | 0.98 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3860 | 1/1   | 0.98 | 0.31 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1758 | 1/1   | 0.98 | 0.20 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3418 | 1/1   | 0.98 | 0.14 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3266 | 1/1   | 0.98 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1760 | 1/1   | 0.98 | 0.19 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3572 | 1/1   | 0.98 | 0.10 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3415 | 1/1   | 0.98 | 0.14 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3264 | 1/1   | 0.98 | 0.64 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3133 | 1/1   | 0.98 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3536 | 1/1   | 0.98 | 0.19 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3135 | 1/1   | 0.98 | 0.13 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3537 | 1/1   | 0.98 | 0.18 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1764 | 1/1   | 0.98 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3474 | 1/1   | 0.98 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3424 | 1/1   | 0.98 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3006 | 1/1   | 0.98 | 0.54 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3276 | 1/1   | 0.98 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3965 | 1/1   | 0.98 | 0.20 | 10,10,10,10                 | 0     |
| 54  | MG   | 2A    | 3278 | 1/1   | 0.98 | 0.10 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3006 | 1/1   | 0.98 | 0.17 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3967 | 1/1   | 0.98 | 0.15 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3774 | 1/1   | 0.98 | 0.10 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3540 | 1/1   | 0.98 | 0.14 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3145 | 1/1   | 0.98 | 0.63 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3776 | 1/1   | 0.98 | 0.13 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3971 | 1/1   | 0.98 | 0.13 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3076 | 1/1   | 0.98 | 0.36 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3477 | 1/1   | 0.98 | 0.16 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3694 | 1/1   | 0.98 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3874 | 1/1   | 0.98 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3243 | 1/1   | 0.98 | 0.13 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3336 | 1/1   | 0.98 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3614 | 1/1   | 0.98 | 0.16 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3480 | 1/1   | 0.98 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3616 | 1/1   | 0.98 | 0.23 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3199 | 1/1   | 0.98 | 0.66 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3378 | 1/1   | 0.98 | 0.09 | 20,20,20,20                 | 0     |
| 54  | MG   | 2A    | 3605 | 1/1   | 0.98 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3026 | 1/1   | 0.98 | 0.42 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3788 | 1/1   | 0.98 | 0.16 | 23,23,23,23                 | 0     |
| 54  | MG   | 2T    | 3002 | 1/1   | 0.98 | 0.11 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3269 | 1/1   | 0.98 | 0.15 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3985 | 1/1   | 0.98 | 0.35 | 36,36,36,36                 | 0     |
| 54  | MG   | 2V    | 201  | 1/1   | 0.98 | 0.16 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3452 | 1/1   | 0.98 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3270 | 1/1   | 0.98 | 0.12 | 11,11,11,11                 | 0     |
| 54  | MG   | 1a    | 1670 | 1/1   | 0.98 | 0.22 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3005 | 1/1   | 0.98 | 0.17 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3136 | 1/1   | 0.98 | 0.20 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3431 | 1/1   | 0.98 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3553 | 1/1   | 0.98 | 0.14 | 18,18,18,18                 | 0     |
| 54  | MG   | 2A    | 3617 | 1/1   | 0.98 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3169 | 1/1   | 0.98 | 0.35 | 38,38,38,38                 | 0     |
| 54  | MG   | 1Q    | 203  | 1/1   | 0.98 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3890 | 1/1   | 0.98 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3627 | 1/1   | 0.98 | 0.26 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3311 | 1/1   | 0.98 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3996 | 1/1   | 0.98 | 0.40 | 27,27,27,27                 | 0     |
| 59  | ZN   | 14    | 501  | 1/1   | 0.98 | 0.14 | 80,80,80,80                 | 0     |
| 59  | ZN   | 15    | 101  | 1/1   | 0.98 | 0.20 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3432 | 1/1   | 0.98 | 0.23 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3625 | 1/1   | 0.98 | 0.12 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3489 | 1/1   | 0.98 | 0.14 | 21,21,21,21                 | 0     |
| 54  | MG   | 2a    | 1609 | 1/1   | 0.98 | 0.17 | 46,46,46,46                 | 0     |
| 60  | SF4  | 1d    | 302  | 8/8   | 0.98 | 0.17 | 48,59,66,72                 | 0     |
| 60  | SF4  | 2d    | 501  | 8/8   | 0.98 | 0.14 | 61,71,81,92                 | 0     |
| 54  | MG   | 1A    | 3511 | 1/1   | 0.99 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3843 | 1/1   | 0.99 | 0.23 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3461 | 1/1   | 0.99 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1716 | 1/1   | 0.99 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 1a    | 1638 | 1/1   | 0.99 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3298 | 1/1   | 0.99 | 0.18 | 14,14,14,14                 | 0     |
| 54  | MG   | 1A    | 3657 | 1/1   | 0.99 | 0.29 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3769 | 1/1   | 0.99 | 0.17 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3620 | 1/1   | 0.99 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3365 | 1/1   | 0.99 | 0.23 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3323 | 1/1   | 0.99 | 0.14 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3034 | 1/1   | 0.99 | 0.10 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3003 | 1/1   | 0.99 | 0.16 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 4004 | 1/1   | 0.99 | 0.25 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3420 | 1/1   | 0.99 | 0.17 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3091 | 1/1   | 0.99 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3661 | 1/1   | 0.99 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3879 | 1/1   | 0.99 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3683 | 1/1   | 0.99 | 0.14 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3585 | 1/1   | 0.99 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | 2E    | 304  | 1/1   | 0.99 | 0.13 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3081 | 1/1   | 0.99 | 0.43 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3009 | 1/1   | 0.99 | 0.20 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3117 | 1/1   | 0.99 | 0.17 | 39,39,39,39                 | 0     |
| 54  | MG   | 1V    | 202  | 1/1   | 0.99 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3625 | 1/1   | 0.99 | 0.10 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3828 | 1/1   | 0.99 | 0.15 | 13,13,13,13                 | 0     |
| 54  | MG   | 1A    | 3915 | 1/1   | 0.99 | 0.11 | 25,25,25,25                 | 0     |
| 54  | MG   | 1B    | 220  | 1/1   | 0.99 | 0.15 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3016 | 1/1   | 0.99 | 0.49 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3650 | 1/1   | 0.99 | 0.16 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 4014 | 1/1   | 0.99 | 0.40 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3645 | 1/1   | 0.99 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3221 | 1/1   | 0.99 | 0.51 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3420 | 1/1   | 0.99 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3243 | 1/1   | 0.99 | 0.15 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3017 | 1/1   | 0.99 | 0.36 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3084 | 1/1   | 0.99 | 0.21 | 33,33,33,33                 | 0     |
| 55  | K    | 1A    | 3287 | 1/1   | 0.99 | 0.06 | 27,27,27,27                 | 0     |
| 55  | K    | 2A    | 3246 | 1/1   | 0.99 | 0.11 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3003 | 1/1   | 0.99 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3442 | 1/1   | 0.99 | 0.16 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3170 | 1/1   | 0.99 | 0.26 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3054 | 1/1   | 0.99 | 0.12 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3787 | 1/1   | 0.99 | 0.23 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3027 | 1/1   | 0.99 | 0.13 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3346 | 1/1   | 0.99 | 0.21 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3895 | 1/1   | 0.99 | 0.11 | 16,16,16,16                 | 0     |
| 54  | MG   | 1D    | 304  | 1/1   | 0.99 | 0.18 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3117 | 1/1   | 0.99 | 0.26 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3740 | 1/1   | 0.99 | 0.18 | 29,29,29,29                 | 0     |
| 59  | ZN   | 1Y    | 501  | 1/1   | 0.99 | 0.20 | 46,46,46,46                 | 0     |
| 54  | MG   | 1D    | 306  | 1/1   | 0.99 | 0.15 | 11,11,11,11                 | 0     |
| 54  | MG   | 2A    | 3257 | 1/1   | 0.99 | 0.18 | 43,43,43,43                 | 0     |
| 59  | ZN   | 16    | 501  | 1/1   | 0.99 | 0.27 | 46,46,46,46                 | 0     |
| 59  | ZN   | 19    | 501  | 1/1   | 0.99 | 0.23 | 39,39,39,39                 | 0     |
| 59  | ZN   | 1n    | 501  | 1/1   | 0.99 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3560 | 1/1   | 0.99 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3309 | 1/1   | 0.99 | 0.10 | 34,34,34,34                 | 0     |
| 59  | ZN   | 25    | 501  | 1/1   | 0.99 | 0.22 | 44,44,44,44                 | 0     |
| 59  | ZN   | 26    | 501  | 1/1   | 0.99 | 0.18 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3403 | 1/1   | 0.99 | 0.29 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3601 | 1/1   | 0.99 | 0.14 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3994 | 1/1   | 0.99 | 0.31 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3869 | 1/1   | 0.99 | 0.14 | 56,56,56,56                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.